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Local atomic and electronic structure of Au-adsorbed Ge(001) surfaces: Scanning tunneling microscopy and x-ray photoemission spectroscopy

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Local atomic and electronic structures of the Au-adsorbed Ge(001) surface are investigated using scanning tunneling microscopy (STM) and x-ray photoemission spectroscopy (XPS). In the STM image, the top of the one-dimensional chain structure of this surface shows an eightfold arrangement of protrusions in the chain direction. The XPS results indicate an absence of buckled Ge-Ge dimers with dangling bonds on the surface. These are inconsistent with any existing structural models assuming a twofold symmetry in the chain direction. An eightfold modulation of the local density of states in the chain direction was observed by STM for an energy region between −0.2 and +0.6 eV from Fermi energy, where a surface metallic band in the occupied state was confirmed by angle-resolved photoemission spectroscopy. Therefore, the metallic surface-state band should follow the eightfold periodicity in the chain direction, contrary to the previous assumption of twofold periodicity.

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I. INTRODUCTION

One-dimensional (1D) structures often appear on metal-adsorbed semiconductor surfaces, where we can expect interesting low-dimensional electronic properties. Among various systems with 1D structures, metallic systems have attracted much attention because of their unique phase transitions such as the Luttinger liquid and charge density wave.[1] Metallic 1D states have been reported in several systems, including Si(557), (553)-Au,[2] and Si(111)-In,[3] while two-dimensional (2D) metals[4,5] and insulators[6] exist on metal-adsorbed semiconductor surfaces with 1D atomic structures.

Recently, the gold-adsorbed Ge(001) surface[7–15] has been identified as one of the systems with 1D atomic structures and metallic surface bands. This surface consists of chains in the ⟨110⟩ direction, which is the same direction as the dimer-row direction on the clean Ge(001) surface. Scanning tunneling microscopy (STM) has confirmed[7–13,16] that the period of the chain in the perpendicular direction is 1.6 nm, which is quadruple the length of the substrate Ge(001)1 × 1 lattice constant. However, the symmetry of the surface structure was not determined by STM because the details of the apparent surface corrugations in the chain direction depend on the sample bias voltage (V_b) and the STM tip condition. Instead, the surface periodicity was classified as 4 × 2 or $c(8 \times 2)$ on the basis of low-energy electron diffraction (LEED),[7,9] leading to the assumption that the periodicity in the chain direction is twice the 1 × 1 lattice constant. In a later LEED study,[11] the additional spots that do not belong to 4 × 2 or $c(8 \times 2)$ periodicity were observed. So far, Au-adsorbed surfaces have consisted of two domains, which makes it difficult to determine the surface superstructure from the available LEED data.

Three models have been proposed for the structure of the chain based on STM observations. The surface suggested by Wang *et al.*[7] consists of Au-Ge and Ge-Ge dimers. In the second model,[9] the top of the chain is made of gold atoms, while it is a chain of Ge-Ge dimers in the third model.[10] In these models, an eightfold periodicity occurs in the direction perpendicular to the chain, while a twofold periodicity is assumed to be in the chain direction. However, an eightfold modulation in the chain direction was later found in STM images at room temperature (RT).[11] Very recently, possible surface structures were theoretically discussed using the results of first-principles calculations,[14,15] and 4 × 2 or $c(8 \times 2)$ models consistent with the existing STM data were not proposed. Thus, the surface atomic structure has not been well understood.

The band structure of this surface was studied by angle-resolved photoemission spectroscopy (ARPES). A metallic surface state was found and its bottom energy is ∼0.2 eV below the Fermi energy (E_F).[9,11] The position of the band bottom was assigned at the zone boundaries ($\bar{J}$ points) of the $c(8 \times 2)$ surface Brillouin zone (SBZ).[11] It strongly disperses in the 4× or 8× direction, perpendicular to the direction with twofold periodicity on the 4×2 or $c(8\times2)$ surface. Whether the metallic surface band is 1D[9] or 2D[11] is a controversial issue. Scanning tunneling spectroscopy (STS) measurements[9] have revealed metallic behaviors on the chain but semiconducting ones between the chains, supporting a 1D chain structure. However, more recent STS measurements on the chain were the same[12,16] as those between the chains, supporting a 2D electronic state. The latter is consistent with the ARPES results showing an anisotropic 2D Fermi surface and the measured dispersions in the two perpendicular directions, ⟨110⟩ and ⟨1$\bar{1}$0⟩.[11] The ARPES measurements were obtained from surfaces with two different domains with chain directions perpendicular to one another. Consequently, the surface Brillouin zone has not been clearly determined from the existing ARPES data, and should be refined with more detailed surface structure information. Both the atomic structure including the eightfold direction and the dimensionality of electronic states are still under debate in this system.

In the present study, we have investigated the Au-adsorbed Ge(001) surfaces that are fully or partially covered by the chains using STM and XPS. Contrary to existing structural models, we have identified an eightfold periodicity of a zigzag structure and a chevron unit in the chain direction. When V_b was between −0.3 V and +0.6 V, the spatial modulation of the local density of states had the same periodicity in the chain direction, indicating that the surface state observed by ARPES has an eightfold periodicity in the chain direction.

II. EXPERIMENTAL

Images were obtained at RT and 80 K using two independent ultra-high-vacuum STMs. All images were acquired in a constant-current mode with an electrochemically etched tungsten tip. For the XPS study of Ge 3*d* core level, we used a hemispherical analyzer at BL18A of Photon Factory, KEK. The incident photon energy was 90 eV and the photoemission angle was 60° from the surface normal. The sample temperature was 80 K. Each chamber for STM and XPS measurements was attached to a sample-preparation chamber, and the base pressure of these chambers was kept below 1×10^{-10} Torr.

The Ge(001) substrate was cut from an n-type Ge(001) wafer (Sb–doped, 0.2–0.4 Ω cm). We introduced the substrate into each sample-preparation chamber, where a clean Ge(001) surface was obtained by repeated cycles of 1-keV Ar^+ sputtering for 20 min and annealing at 950 K for 20 min. Gold was deposited from a tungsten basket onto the clean Ge(001) surface kept at RT or 670 K. A well-ordered surface with the chain structures was formed by deposition at 670 K, while the chain structure was also formed by deposition at RT followed by annealing at 670 K as reported in Ref. 8.

III. RESULTS AND DISCUSSION

Figure 1 shows typical RT-STM images of the Au-adsorbed Ge(001) surface with the chains. As previously observed,[13] a zigzag protrusion is seen at the top of the chain for $V_b = -0.6$ V while it is absent for $V_b = +1.0$ V. The zigzag protrusion is observed for $-1.5\ \text{V} \leqq V_b \leqq -0.5$ V at RT.

We measured the sample-bias dependence of the STM images at 80 K for $-1.0\ \text{V} \leqq V_b \leqq +1.0$ V. Part of the results are shown in Fig. 2. For $V_b = -0.5$ V, the image is similar to that shown in Fig. 1(b). For $-0.3\ \text{V} \leqq V_b \leqq +0.6$ V, an apparent height modulation of the STM images is seen in the chain direction with an averaged period of 3.2 nm, 8 times the surface lattice constant.

The eightfold periodicity in the chain direction is demonstrated as (0,1/8) spots in the fast Fourier transformation (FFT) of the STM image for $V_b = -0.1$ V as shown in Fig. 3(a). The (0,1/8) spot is missing in the FFT-STM image for $V_b = -0.5$ V (Fig. 3(b)). Here, we rotate the images to make the chain direction to be vertical. A (1/4,0) peak indicates that the periodicity in the direction perpendicular to the chain is present at both $V_b = -0.1$ and -0.5 V. A quantitative analysis of the peaks is, however, difficult because of the considerable background noise. There has been no report on the eightfold periodicity in the chain direction except the FFT-STM image taken at RT for $V_b = -1.2$ V.[11]

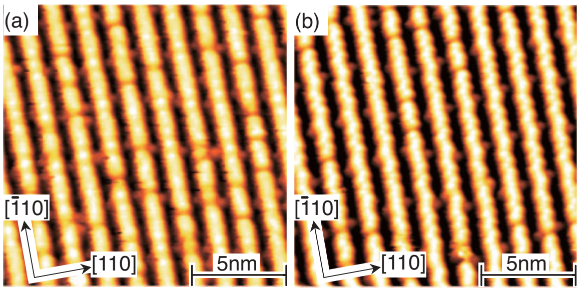

FIG. 1. (Color online) STM images of the Au-adsorbed Ge(001) surface with chains at RT for (a) $V_b = +1.0$ V and (b) $V_b = -0.6$ V.

The height modulation in the chain is weakly correlated with those of the adjacent chains as in Fig. 2. The peak of the modulation in the adjacent chain often shifts slightly in the chain direction. However, the direction and amount of shift are irregular, and the local periodicity of the modulation can differ in the adjacent chain. Therefore, there is no long-range order of the height modulation in the direction perpendicular to the chain.

The observed eightfold modulation in the STM images for $-0.3\ \text{V} \leqq V_b \leqq -0.1$ V is attributed to the surface metal band that was found below E_F in the previous ARPES studies. This state exists in the bulk band gap and has its bottom at ~0.2 eV below E_F. Our STM results indicate that the density of states of this surface state has the eightfold modulation in the chain direction. The surface state should continue above E_F because modulation with the same period was observed in the STM images for the positive V_b below +0.6 V as in Fig. 2.

In order to determine the relationship between atomic structure and the modulation of the electronic states, we analyzed a high-resolution STM image that shows atomic-size protrusions on the chain top [Fig. 4(a)]. There is no definite long-range order in the arrangement of the protrusion. However, we can see local zigzag structures and a chevron unit of the protrusions. There are characteristic combinations of the chevron unit and the zigzag structure with different lengths, which are labeled lines A–C in Fig. 4(a). Schematic models of these combinations are given in Fig. 4(b). Model B occurs most frequently on the surface. The variety of zigzag length introduces disorders to the surface structure. Adjacent zigzag structures occasionally form a very local $c(8 \times 2)$ unit [Fig. 4(a)], but this structure does not cover the whole surface contrary to the previous assumption.

When the average coverage of Au on the surface is not enough to cover the whole surface with the chain structure, the resulting surface consists of islands of chains and flat areas without chains.[7,8] In order to make clear the unit length of the surface periodicity, we compared the length of the model B arrangement with the substrate lattice constant on the surface that was partially covered with the Au-induced chains. Protrusions of Ge dimer size similar to those found on a clean Ge surface and defects were seen on the flat surface without the Au-induced chains, and the surface exhibited no long-range structural order as in Fig. 5. We refer to these protrusions as dimers, which can be made of Ge or Au atoms. The length of the model B arrangement corresponds to 4 times the dimer width, which is 8 times the 1×1 surface lattice unit (Fig. 5; dashed lines) and is consistent with the eightfold modulation observed by STM (Fig. 2). The length of the chevron unit observed by STM, that is, the length between protrusion α and protrusion β in model B [Fig. 4(b)], is 10 % longer than that of the zigzag structure between β and γ. It should be noted that the observed position of the protrusion by STM is not always the same as the surface atom position. The relationship between the two should be confirmed by theoretical study with a proper structural model.

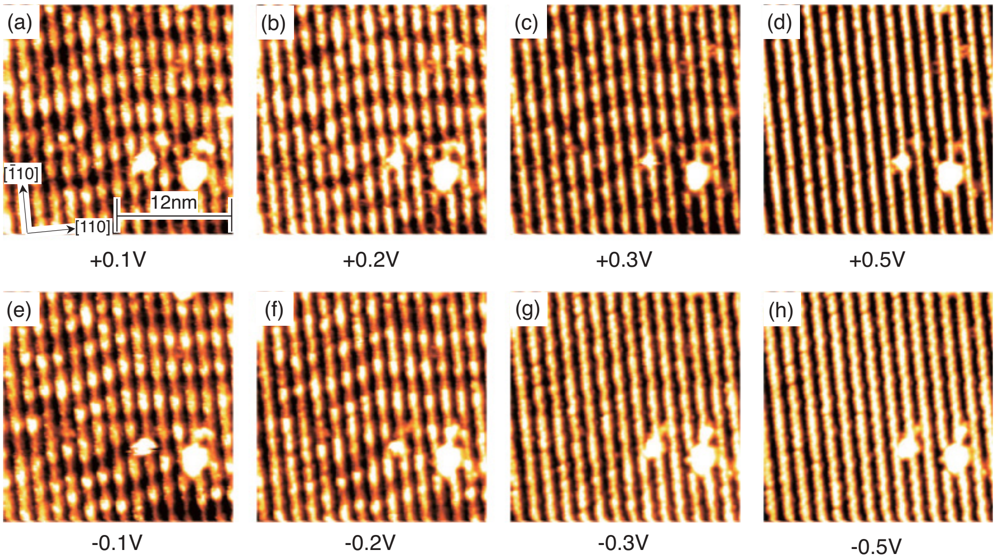

FIG. 2. (Color online) Sample-bias (V_b) dependence of the STM images of the Au-adsorbed Ge(001) surface with chains at 80 K. Values of V_b are given in the figure. The tunneling current was commonly 0.5 nA.

The distribution of the different lengths of zigzag structures and the chevron unit for the area shown in Fig. 2 is illustrated in Fig. 6(a). Less than half of the chains on the surface can be categorized by the model structures A–C, with the other areas consisting of the chevron unit, the zigzag structure, and other nonperiodic structures. The apparent height of the chevron unit is smaller than that at the zigzag structure in the magnified image with $V_b = -0.2$ V [Fig. 6(b)], indicating that the local density of states of the surface metallic state of the chevron unit is lower than that of the zigzag structure for the electron energy between E_F and 0.2 eV below E_F. Furthermore, the local density of states is also lower at the chevron unit in the empty state when the electron energy is less than 0.5 eV (Fig. 2). The apparent height at the center protrusion of the chevron unit increases with increasing V_b from +0.2 V [Figs. 2(a)–2(d)] as clearly shown in the magnified images [Figs. 6(c) and 6(d)] for $V_b = +0.1$ and +0.3 V.

Examining a chain island on a flat surface yields important information about the chain structure. If the chain consists of Au-Ge and Ge-Ge dimers as proposed in Wang's model,[7] then it should be on the same terrace as the clean Ge dimers. Figure 7(a) shows an STM image with a chain island and the cross sections along the lines *l*–*n* are given in Fig. 7(b). The terrace T_1 is higher than the terrace T_2 by the single step height of the clean Ge(001) surface as shown in cross section *l*. This height difference is the same between the top of the chain island and the terrace T_1. On the surface without the Au-induced chains, the dimer row direction on a terrace is

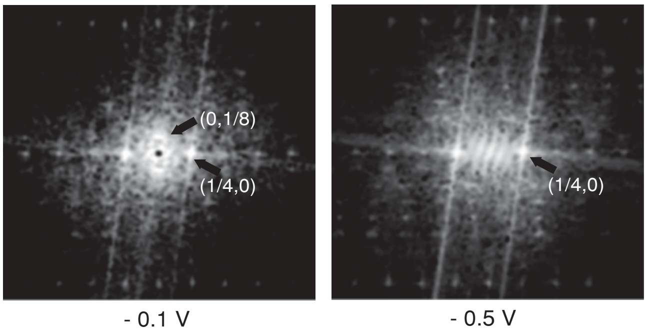

FIG. 3. Central parts of the Fourier-transformed STM images showing the presence (a) and absence (b) of the eightfold periodicity of the STM images in Fig. 2(e) and 2(h), respectively. The sample-bias voltages are given in the figure. The (0, 1/8) peak in (a) indicates the eightfold periodicity in the chain direction. We rotated the images to make the chain direction vertical for clarity.

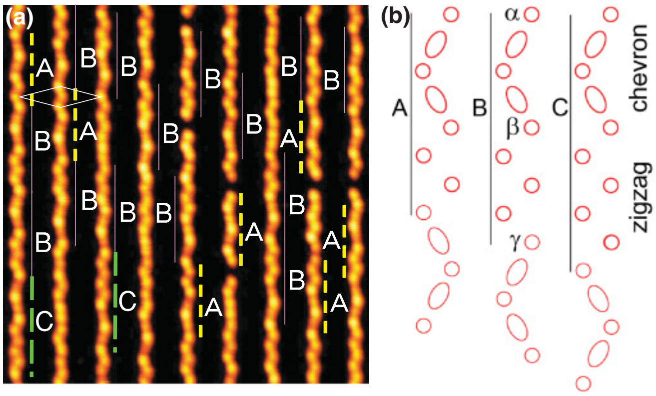

FIG. 4. (Color online) (a) High-resolution STM image showing protrusions on top of the chains on the surface with $V_b = -1.0$ V. The image was taken at 80 K. Typical arrangements of the protrusions in the chain direction are indicated by dotted, solid and dashed lines A–C. They consist of a chevron unit and zigzag structures with different lengths. Among these arrangements, the B type is the most frequently seen on the surface. The length of line B is 3.2 nm. A very local $c(8 \times 2)$ arrangement of the zigzag structure is indicated as the white diamond. (b) Schematic models of the common arrangements of the protrusions consisting of a chevron unit and zigzag structures. Models A–C correspond to arrangements A–C in (a). The total length increases with increasing length of the zigzag structure.

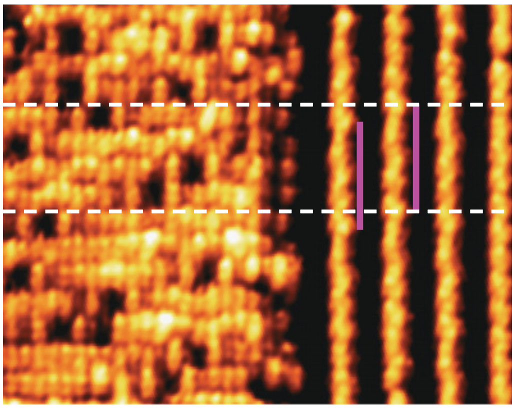

FIG. 5. (Color online) STM image around the boundary between a chain island (right) and an area without chains (left) on the Au-adsorbed Ge(001) surface partially covered with the Au-induced chains. The image was taken at RT with $V_b = -1.0$ V. The image contrast was modified to show the chevron unit and zigzag structures at the top of the chain. Model B arrangements on the chain island are indicated by solid (purple) lines of 3.2 nm. Dashed lines are guides for eye.

perpendicular to that on the adjacent terraces separated by a single step height. However, the relationship between the direction of the dimer row and the Au-induced chains differs since the direction is the same for the terrace T_1 and the chain island while the height is different (Fig. 7). When the height difference is the same as shown in Fig. 5, the chain direction is perpendicular to the dimer-row direction on the terrace without chains. This contradicts the Au-Ge and Ge-Ge dimer model.[7]

The protrusions that we observed in the troughs between the chains (Fig. 1) are similar to those found in previously published STM images,[10,12,13] but they have been ignored up to now. The structure in the trough is important for verifying the proposed facet models.[10,15] They appear to be adjacent to the chevron units, as can be seen more clearly at the boundary of the flat surface shown in Fig. 7(a). The relation between the protrusion and the chevron unit is shown schematically in Fig. 7(c) with a magnified STM image. The protrusion destroys the symmetry of the chevron unit. The arrows in Fig. 7(b) indicate the positions of the protrusions in the cross sections along the line *n*. The apparent height difference between the protrusion in the trough and the top of the chain is 0.12 nm, which is shorter than the single step height on Ge(001). The eightfold periodicity observed in the FFT-STM image at RT[11] was mainly caused by the protrusions in the trough. Unfortunately, it is difficult to obtain reproducible STM images in the trough of anything but the protrusion because the image is largely dependent on the shape of the tip apex.

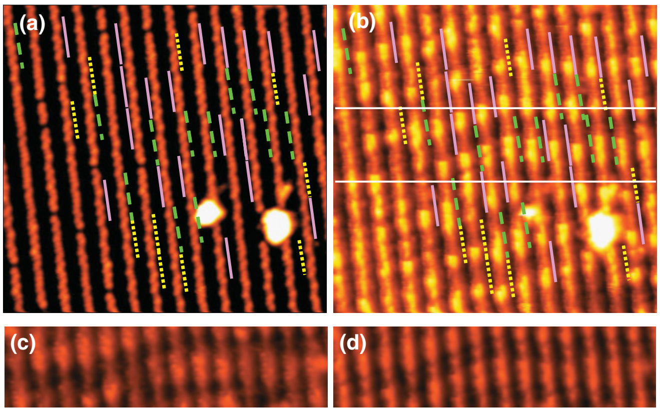

FIG. 6. (Color online) (a,b) STM images of the surface showing arrangements A–C of the chain protrusions for (a) $V_b = -1.0$ V and (b) $V_b = -0.2$ V. The surface is the same as that shown in Fig. 2, and the contrast is modified to show arrangements A–C of the protrusions in (a). Dotted, short solid and dashed lines indicate arrangements A, B and C of the chevron unit and the zigzag structure given in Fig. 4(b), respectively. (c,d) Magnified STM images for (c) $V_b = +0.1$ V and (d) $V_b = +0.3$ V. Imaged areas are the same as that between the two horizontal white lines in (b).

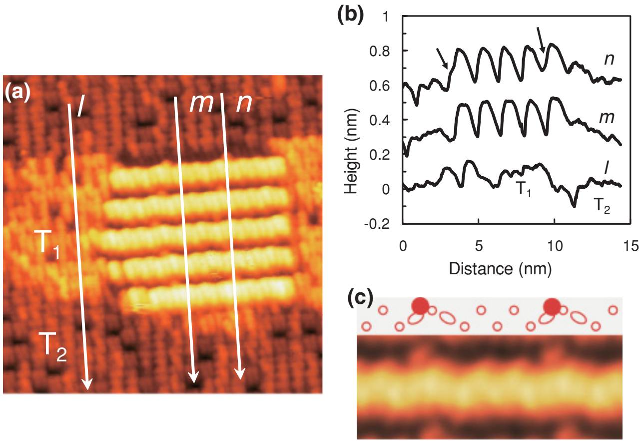

FIG. 7. (Color online) (a) STM image of a chain island on an Au-adsorbed Ge(001) surface partially covered with Au-induced chains. The image was taken at RT with $V_b = -1.0$ V. (b) Cross sections along the lines *l*, *m*, and *n* shown in (a). Line *n* is on the protrusions in the troughs as indicated by arrows. (c) Schematic model showing the relation between the chevron unit and the protrusion in the trough, and corresponding STM image. In the model, open circles are protrusions on the chain, and gray (red) circles protrusions in the trough. The image is magnified from that shown in Fig. 1(b).

It should be noted that previously published results were obtained from surfaces that were prepared differently, particularly regarding the temperature at which the Au was deposited.[7–13] Different methods of preparation may result in variation of the local structure of the chains. Thus, we studied whether the structure of the top of the chain and the presence of the protrusions in the trough depend on the substrate temperature by varying the temperature during Au deposition from 570 to 770 K. The chain structure can be made by Au deposition while the substrate temperature is kept in this range or by annealing at these temperatures after the deposition at RT. Either preparation method results in the protrusions at the top of the chain forming the zigzag structure and the chevron unit with the protrusion in the adjacent trough. Therefore, these atomic structures are independent of the preparation methods.

The zigzag arrangement of the protrusions on the chain suggested the presence of buckled Ge dimers as are found on a clean Ge(001) surface.[7,10] The Ge-Ge dimers with dangling bonds on the clean surface are detected using the Ge 3*d*-core spectra. Figure 8 shows the spectra as a function of the

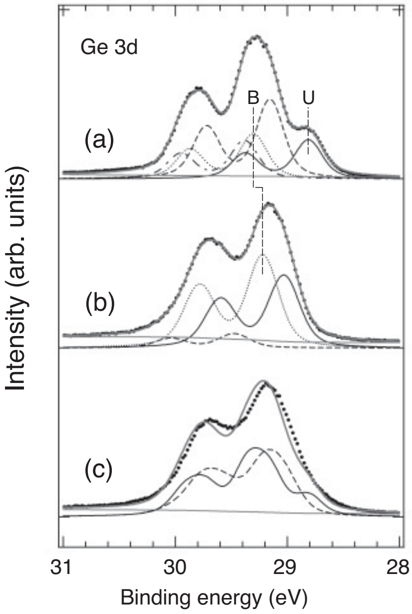

FIG. 8. Ge 3*d* core spectra for (a) a clean Ge(001) surface, (b) a surface fully covered by the Au-induced chain structure, and (c) a surface that is half-covered by the chain structure. Data are shown as filled circles. Spectra were normalized to their integrated intensity after subtraction of the background. Those shown in (a) and (b) were decomposed using Voigt functions. Dotted curves in (a) and (b) are assigned to bulk components (B) since their intensities relative to other components increase in bulk-sensitive measurements. The shift of the binding energy by ∼0.1 eV is due to the different band bending. Solid, dashed and single-dotted, and dashed curves in (a) are assigned to the upper (U) and lower atoms of the buckled dimer and the subsurface atoms, respectively. The sum of these components and the background (gray curve) is shown by the thick gray curve as a fitting result. Solid, dashed, and thick gray curves in (c) correspond to the sums of the fitted components in (a) and (b) with 50% intensity and to their sum, respectively.

binding energy E_B from E_F for the Ge(001) clean surface, a surface fully covered with Au-induced chains, and a surface half-covered with chains. On the clean surface, the peak at $E_B = 28.8$ eV [U in Fig. 8(a)] is attributed to the upper Ge atom of the buckled dimer with a dangling bond.[17] This peak was completely missing for the surface with the Au-induced chains [Fig. 8(b)], clearly indicating the absence of the buckled Ge-Ge dimer with dangling bonds on the surface. On the surface that was only half covered with chains, there is also a peak at $E_B = 28.8$ eV [Fig. 8(c)] from the Ge-Ge dimers on the Au-deposited surface without the chains where a local $c(4 \times 2)$ structure can be seen as evidence for the existence of buckled Ge-Ge dimers.

We deconvoluted these spectra using Voigt functions as done in previous studies[17,18] of the clean surface. The four fitted components of the clean surface are attributed to the upper and lower dimer, subsurface, and bulk atoms [Fig. 8(a)]. For a surface with Au-induced chains, two components were needed to fit the result in addition to the component of the bulk Ge atoms [Fig. 8(b)]. The results of fitting with more than four components were not reliable because the fitted peak energies have large errors. Therefore, we can confirm at least two surface or subsurface components for the fully covered surface. The binding energies of these two components are lower and higher than that of the bulk component. However, the shift of the lower component is smaller than that for the upper Ge atoms of the dimer on the clean surface, indicating a moderate electron transfer for these Ge atoms compared to the buckled Ge-Ge dimers on the clean surface.

It is difficult to deconvolute the spectrum for the half-covered surface [Fig. 8(c)]. It has at least seven components for both the clean surface and chain structures. We attempted to fit the spectrum using the sum of the spectra for the clean and full-covered surfaces but the fitting was not as good as those in Figs. 8(a) and 8(b). The surface without the chain structure contains the clean Ge dimers, but the Au atoms there modify the surface electronic structure and the 3*d* core states of the neighboring Ge atoms.

So far, several models have been proposed for the chain structure, including Au-substituted dimer row models,[7,14] an added Au-wire model,[9] and a model made of (111) facets.[10] Models that include rows of buckled Ge-Ge dimers with dangling bonds are clearly excluded by the preceding XPS results. Au-Au or Au-Ge dimers cannot be made simply by substituting the Ge atoms on the clean surface with Au atoms because the relationship between the chain and dimer row directions shown in Figs. 5 and 7 is inconsistent with this interpretation. The recent theoretical study[15] indicated that added Au-wire models have higher formation energies than Au-substituted dimer row models, and suggested that facet-based models were promising. We have found that the period of the zigzag structure is shorter than twice of the substrate 1×1 lattice unit because of the presence of the elongated chevron unit. A facet structure can reduce the total increase of the lattice energy, which is caused by the lattice distortion due to the presence of the elongated chevron unit at the top of the chain. A simple model with the Ge(111)$\sqrt{3} \times \sqrt{3}$ Au[19] facet is, however, inconsistent with the observed eightfold periodicity in the chain direction.

Previous structural models were based on the surface periodicity of 4×2 or $c(8 \times 2)$ observed by LEED, and twofold symmetry was assumed to occur in the chain direction. However, our STM images indicate an eightfold structure modulation in the chain direction at the top of the chain, and a protrusion adjacent to the chevron unit in the trough. The metallic surface band also has an eightfold modulation of the density of states in the chain direction (Fig. 2). The periodicity of the chain in the direction perpendicular to the chain is four times the 1×1 lattice constant. Thus, the chain structure has a 8×4 periodicity or a larger. It is possible that an atomic structure showing 4×2 or $c(8 \times 2)$ periodicities, as observed by LEED, exists in the trough between the chains, and could not be observed clearly by STM. At present, realistic structural models that can explain the LEED results and the metallic surface state have not been proposed. More complicated structural models are necessary that include the chevron unit with a protrusion in the trough.

IV. CONCLUSION

We have studied the atomic structure of the Ge(001) surface with Au-induced chains by STM and XPS. The top of the chain consists of a chevron unit and a zigzag structure. The former is accompanied by a protrusion in the trough between the chains. The absence of buckled Ge-Ge dimers with dangling bonds in the Au-induced chains was confirmed by XPS. As a consequence of the alternative arrangement of the chevron unit and the zigzag structure in the chain direction, an eightfold periodicity exists in the chain direction. This excludes the existing three structural models just as the results of the first-principles calculation[15] did. The local density of states in the chevron unit is lower than that in the zigzag structure in the energy range close to E_F, where a metallic surface state has been detected by ARPES. This induces an eightfold charge modulation in the same energy range. Consequently, the metallic surface state observed by ARPES has an eightfold periodicity in the chain direction, which is inconsistent with the previously assumed twofold periodicity in this direction. Further structural information on the trough area is needed to understand the detailed atomic and electronic structures of this surface.

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