

## Structure of an InAs(111)A-(2×2)S surface studied by scanning tunneling microscopy, photoelectron spectroscopy, and x-ray photoelectron diffraction

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The structure of an InAs(111)A-(2×2)S surface has been studied by using scanning tunneling microscopy (STM), synchrotron radiation photoemission spectroscopy (SRPES), and x-ray photoelectron diffraction (XPD). Honeycomblike images are observed by STM measured at a bias voltage of  $-1.4$  V. Similar images are also observed at  $+1.5$  V, although the intensity of the alternative corner of a hexagon is depressed, resulting in a threefold symmetry. S 2s and As 3d XPD patterns show that sulfur atoms rarely exchange the fourfold arsenic sites. Three surface components are found in the In 4d spectra. On the other hand, no surface components are found in the As 3d spectra. Based on the STM, SRPES, and XPD results, a probable structure model for the (2×2)S surface is proposed. The experimental XPD patterns are in good agreement with the calculated ones.

### I. INTRODUCTION

Sulfur-adsorbed III-V compound semiconductor surfaces have been extensively studied by various surface-sensitive techniques because electrical properties of the surfaces are tremendously improved.<sup>1</sup> On the other hand, understanding the surface structure in an atomic level is very important for homoepitaxy and heteroepitaxy on the sulfur-adsorbed surfaces, because the epitaxial growth is strongly dependent upon the surface structure of substrates.

For sulfur-treated GaAs, 2×1 (Ref. 2) and 1×1 (Ref. 3) reconstructions were found for (001) and (111) surfaces, respectively. It was reported that sulfur is bridged to Ga atoms to form the 2×1 structure.<sup>4,5</sup> The photoelectron spectra (PES) and scanning tunneling microscopy (STM) results suggested that S-S dimer is formed on the 4×1 surface.<sup>5</sup> On the other hand, formation of the dimer lining up in the  $[\bar{1}10]$  direction was not confirmed by soft-x-ray standing wave (XSW) method.<sup>4</sup> Based on the above results, two models for the 2×1 reconstruction can be assumed: One is the model that sulfur is bridged on alternative Ga atoms in the  $[110]$  direction, and the other model that sulfur is bridged on all Ga atoms in the  $[110]$  direction, forming a S-S dimer in the  $[\bar{1}10]$  direction. The sulfur coverages are 0.5 and 1.0 ML for the former and latter models, respectively. It was suggested by XSW (Ref. 6) and PES (Ref. 7) results that sulfur is adsorbed on Ga atoms at the (111)A surface and exchanges As at the (111)B to form the 1×1 structure. The 2×6 reconstruction prepared by H<sub>2</sub>S adsorption was also reported.<sup>8</sup>

The 2×1 reconstruction was also found for sulfur-adsorbed GaP(001) (Ref. 9) and InP(001) (Refs. 10 and 11) surfaces, although it was reported to be the 1×2 surface (Refs. 9 and 11) because the cation-stabilized surface structure was understood to be the 4×2 reconstruction at that time. Since the sulfur coverage was found to be about 0.5 ML,<sup>10</sup> sulfur could be bridged on In(Ga) in the  $[110]$  direc-

tion, being in good agreement with STM result.<sup>12</sup> Although the 1×1 structure was found on the InP(001) surface,<sup>13</sup> a reconstruction with a sulfur coverage about 1 ML was ascribed to the 2×1 structures based on the STM, low-energy electron-diffraction (LEED), and x-ray photoelectron spectroscopy (XPS) results.<sup>12</sup>

The 2×1 and 1×1 reconstructions were reported for the sulfur-adsorbed InAs(001) (Ref. 14) and (111)B (Ref. 15) surfaces, respectively, which is the same result as for GaAs. However, recently we found the 2×2 reconstruction for the sulfur-adsorbed InAs(111)A surface.<sup>14</sup> This is completely different from the reconstruction which was reported on the sulfur-adsorbed III-V compound semiconductor surfaces. Therefore, we have studied the 2×2 surface in detail with STM, synchrotron radiation photoemission spectroscopy (SRPES), and x-ray photoelectron diffraction (XPD). A probable model for the InAs(111)A-(2×2)S surface will be proposed.

### II. EXPERIMENT

An *n*-type InAs(111) sample (carrier density,  $3 \times 10^{17}/\text{cm}^3$ ) was used. Preparation of the InAs(111)A-(2×2)S surface was described elsewhere.<sup>15</sup> No contaminants such as carbon and oxygen were detected by XPS. The surface structure was confirmed by a clear 2×2 LEED pattern.

STM measurements were performed using a JSTM-4500XT system (JEOL). STM images were measured with an electrochemically polished tungsten tip at two sample biases ( $V_s$ ) of  $-1.4$  and  $+1.5$  V. XPD measurements were performed using an angle-resolved electron spectrometer system (ADES-400, VG Scientific) where the acceptance angle of photoelectrons was  $\pm 2^\circ$ . S 2s and As 3d photoelectron intensities were measured by using a Mg  $K\alpha$  (1253.6 eV) source. The azimuthal angle  $\phi=0^\circ$  in the photoemission direction for the sample was set in the  $[\bar{1}\bar{1}2]$  direction

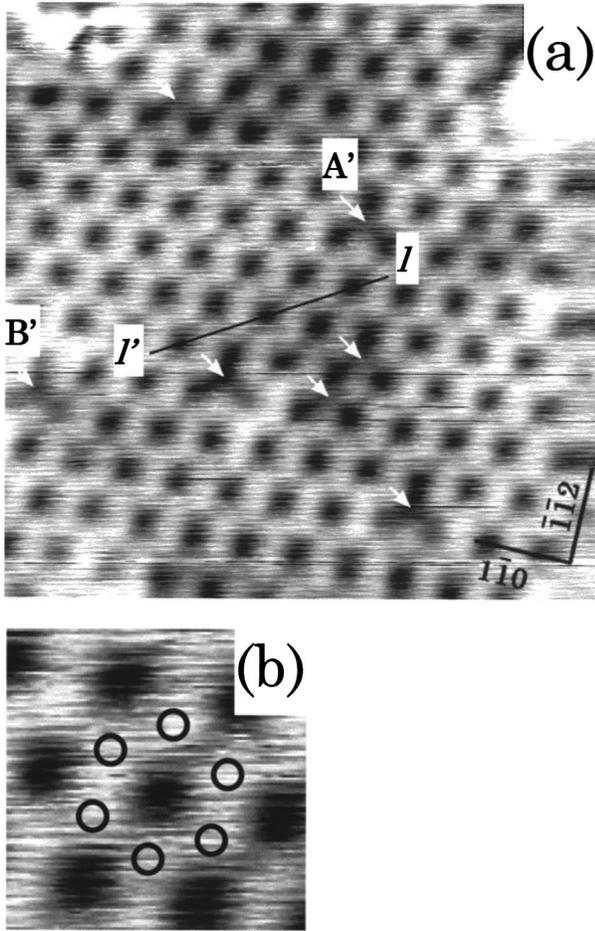


FIG. 1. A STM image (a) and the magnified image (b) of the InAs(111)A-(2×2)S surface measured at bias voltage of  $V_s = -1.4$  V. The image sizes in (a) and (b) are  $10 \times 10$  and  $2.2 \times 2.2$  nm, respectively. Arrows in (a) indicate the defects on the surface. Open circles in (b) correspond to the corners of the hexagon.

SRPES measurements were performed at the vacuum ultraviolet (VUV) beam line (BL18A) of Photon Factory at KEK (Tsukuba, Japan). Photons of 80 and 100 eV were used for the measurements of In 4*d* and As 3*d* spectra, respectively. XPD, STM, and SRPES measurements were carried out in a better vacuum than  $1 \times 10^{-8}$  Pa.

### III. RESULTS

A STM image of the (111)A-(2×2)S surface measured at a bias voltage of  $-1.4$  V is shown in Fig. 1(a), where the images of a honeycomb shape are observed. The nearest distance between the holes of the hexagons in the  $[1\bar{1}0]$  direction is about 0.86 nm, being in accordance with two times of the distance between {110} planes of InAs. Figure 1(b) shows the magnified image of the honeycomb structure observed in (a). The height of protrusions corresponding to the corners of the hexagon is almost equal, resulting in a sixfold symmetric structure.

The STM image measured at a bias voltage of  $+1.5$  V is shown in Fig. 2(a), where the  $2 \times 2$  honeycomb structure is also seen. However, as shown in Fig. 2(b), the intensity of

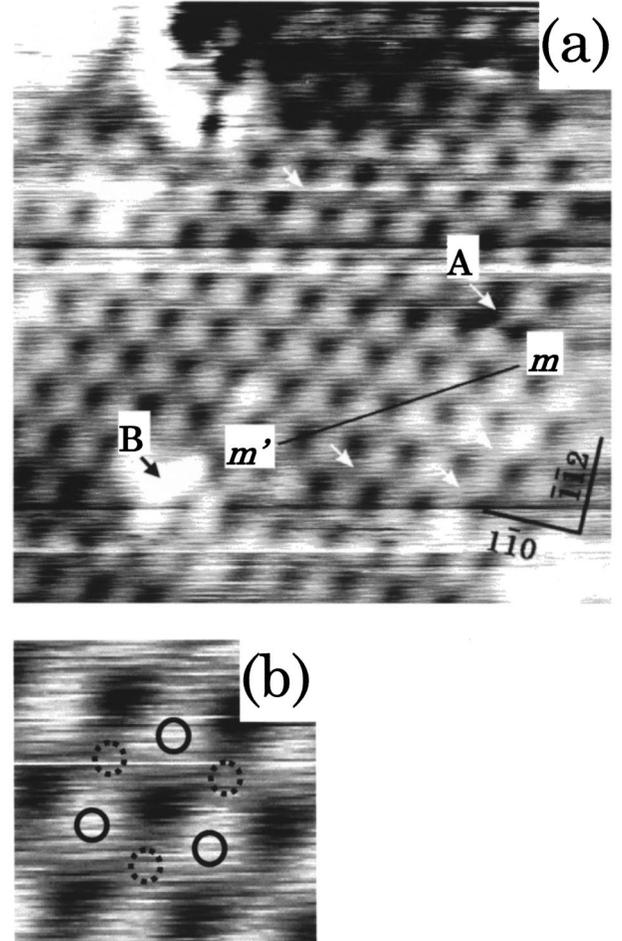


FIG. 2. A STM image (a) and the magnified image (b) of the InAs(111)A-(2×2)S surface measured at bias voltage of  $V_s = +1.5$  V. The image sizes in (a) and (b) are  $10 \times 10$  and  $2.2 \times 2.2$  nm, respectively. Arrows in (a) correspond to the defects in Fig. 1(a). Both solid and broken circles in (b) correspond to the corners of the hexagon. The protrusions indicated by the broken circles are located lower than those indicated by the solid ones.

the protrusions corresponding to the corners of the hexagon is alternatively depressed, resulting in a threefold-symmetric structure. Since a band at about  $+1.5$  eV above the Fermi level in an inverse photoemission spectrum (IPES) for the (2×2)S surface was ascribed to unoccupied dangling bond states of surface indium atoms,<sup>15</sup> the STM image shown in Fig. 2 represents a contour of the states.

Line profiles along 1-1' [Fig. 1(a)] and  $m$ - $m'$  [Fig. 2(a)], which are in the  $[211]$  direction, are shown in Figs. 3(a) and 3(b), respectively. It is found that the distance between the two protrusions corresponding to a neighboring corner of the hexagon is about 0.5 nm, and that the depth of a center hole in the hexagon is about 0.1 nm. It is also found from profile (b) that the difference in height between the nearest corners is about 0.03 nm.

Some defects are observed at a negative bias [arrows in Fig. 1(a)]. Comparing Figs. 1(a) and 2(a), all the defects observed at the negative bias correspond to the low-intensity corners of the hexagon in Fig. 2(a) (arrows). The defects are not always observed at a positive bias, although the defect A and bump B, which correspond to the defects A' and B',

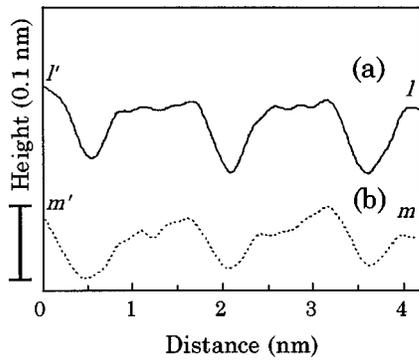


FIG. 3. Line profiles along the lines 1–1' (a) and  $m$ – $m'$  (b) shown in Figs. 1 and 2, respectively. Both profiles trace the same line on the surface.

respectively, in Fig. 1(a), are observed in Fig. 2(a).

Figure 4 shows  $S 2s$  [(a)–(c)] and  $As 3d$  (d) XPD azimuthal patterns for the surface. These patterns were measured at polar angles of  $63^\circ$  (a),  $71^\circ$  [(b) and (d)], and  $78^\circ$  (c). A strong peak appears for the  $As 3d$  pattern at  $\phi = 60^\circ$ , that is, the  $[\bar{2}11]$  direction. The peak originates from forward scattering of  $As 3d$  photoelectrons by nearest In atoms in the  $[\bar{1}11]$  direction. A large anisotropy is observed at about  $\phi = 0^\circ$  and  $60^\circ$  for the  $S 2s$  patterns measured at the polar angles of  $\theta = 71^\circ$ ,  $78^\circ$ , and  $63^\circ$ , respectively. The large anisotropy at  $\phi = 60^\circ$  does not appear at  $\theta = 71^\circ$  for the  $S 2s$  pattern while it was found for the  $As 3d$  pattern at  $\theta = 71^\circ$ , indicating that no strong scatterers for  $S 2s$  photoelectrons exist in the  $[\bar{1}11]$  direction. This implies that most of the sulfur atoms do not occupy the fourfold arsenic sites in the bulk.

Figure 5 shows  $S 2s$  XPD polar patterns for the surface measured at azimuthal angles of  $0^\circ$  and  $60^\circ$ . Since the pho-

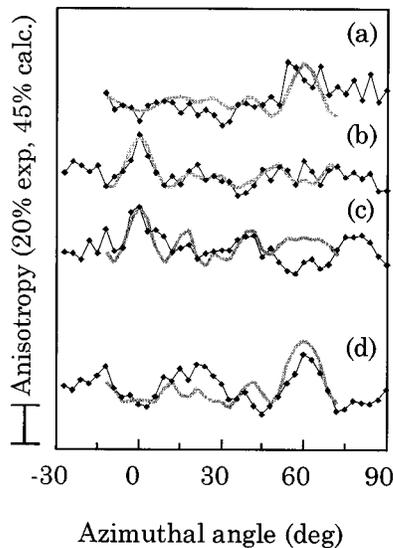


FIG. 4.  $S 2s$  (a)–(c) and  $As 3d$  (d) azimuthal XPD patterns for the  $InAs(111)A-(2 \times 2)S$  surface. Anisotropy, i.e., relative intensity to the maximum intensity, are plotted as a function of the azimuthal angle  $\phi$ . The patterns measured at  $\theta = 63^\circ$  (a),  $71^\circ$  [(b) and (d)], and  $78^\circ$  (c), off the normal to the surface, are displayed by dots with solid lines. The patterns calculated using the single scattering procedure are superimposed on the measured ones (shaded lines).

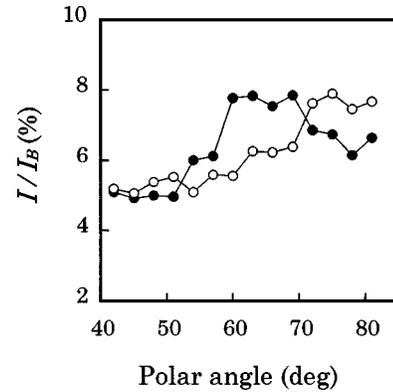


FIG. 5.  $S 2s$  polar XPD patterns for the  $InAs(111)A-(2 \times 2)S$  surface measured at  $\phi = 0^\circ$  (open) and  $60^\circ$  (filled). The photoemission intensity to the background is plotted as a function of  $\theta$ .

toemission intensity depends upon the detection angles, the intensity ratio  $I/I_B$  is used as the anisotropy. Here  $I$  and  $I_B$  correspond to the  $S 2s$  and background intensities, respectively. The large anisotropy is observed at  $\theta = 71^\circ$ – $81^\circ$  ( $60^\circ$ – $69^\circ$ ) for the pattern measured at  $\phi = 0^\circ$  ( $60^\circ$ ). This is consistent with the  $S 2s$  azimuthal patterns shown in Fig. 4. Since the large anisotropy appears at  $\theta = 60^\circ$ – $69^\circ$  for  $\phi = 60^\circ$ , the sulfur atoms do not exist at the first layer of the surface.

In  $4d$  spectra for the surface measured at detection angles of  $80^\circ$  (a) and  $0^\circ$  (b) are shown in Fig. 6. The curve fitting by a Voigt function<sup>16</sup> and various parameters for the fitting are shown in the spectra and Table I, respectively. Three doublet components of  $S1$ ,  $S2$ , and  $S3$ , and a bulk component  $B$  are found. The binding energies (BE's) of  $S1$ ,  $S2$ , and  $S3$  are shifted by  $+0.58$ ,  $+0.30$ , and  $-0.60$  eV, respectively, from the bulk component. Since the relative intensities of  $S1$ ,  $S2$ , and  $S3$  to that of the bulk component are increased at the high detection angle, these components can be ascribed to indium atoms located at the surface. The intensity ratios of  $S1/B$ ,  $S2/B$ , and  $S3/B$  are 0.53, 0.71, and 0.11, respectively,

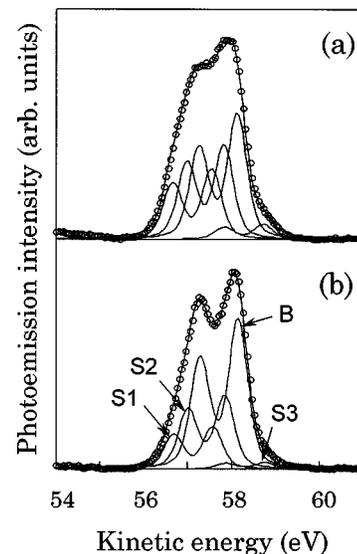


FIG. 6. In  $4d$  spectra for the  $InAs(111)A-(2 \times 2)S$  surface measured at detection angles of  $80^\circ$  (a) and  $0^\circ$  (b) off the normal to the surface. The spectra were measured at a photon energy of 80 eV.

TABLE I. The curve-fitting parameters for In 4*d* spectra.

Components	<i>B</i>	<i>S1</i>	<i>S2</i>	<i>S3</i>	
Relative intensity	$\theta=0^\circ$	1	0.27	0.46	0.04
	$\theta=80^\circ$	1	0.53	0.71	0.11
Branching ratio	$\theta=0^\circ$	1.36	1.23	1.23	1.17
	$\theta=80^\circ$	1.37	1.26	1.23	1.23
Spin-orbit splitting (eV)	0.87	0.89	0.84	0.89	
BE shift (eV)	0	0.58	0.30	-0.60	
Lorentzian width (eV)	0.20	0.20	0.20	0.20	
Gaussian width (eV)	0.41	0.41	0.41	0.41	

at the detection angle of  $80^\circ$ , where the escape depth of the photoelectron is estimated to be 0.1–0.2 nm. The intensity ratio of *S3/B* is too small to be ascribed to the principal indium atoms which constitute the  $(2\times 2)S$  surface structure.

As 3*d* spectra for the surface measured at detection angles of  $80^\circ$  (a) and  $0^\circ$  (b) are shown in Fig. 7. Only one doublet component is found to be fitted for both spectra. The fitting parameters are as follows: the Gaussian and Lorentzian widths are 0.5 and 0.075 eV, respectively; and the spin-orbit splitting is 0.69 eV. The surface core-level shift of As 3*d* photoelectrons is not found for the surface. This doublet component can be ascribed to arsenic in the bulk.

#### IV. DISCUSSION

Based on the STM, XPD, and SRPES results described above, as well as the XPS and IPES results,<sup>15</sup> a structure model for the InAs(111)A-(2×2)S surface is proposed in Fig. 8. The first and second layers in the model are occupied by In and S atoms, respectively, forming a honeycomb structure in which the length between the nearest protrusions is suggested to be about 0.5 nm from the STM results. The indium atoms at the first layer are bonded to sulfur at the second layer, and they are in a threefold coordination, result-

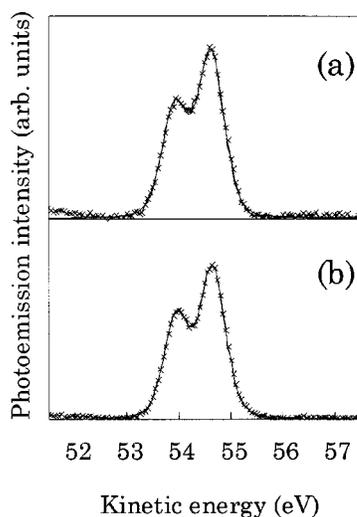


FIG. 7. As 3*d* spectra for the InAs(111)A-(2×2)S surface measured at detection angles of  $80^\circ$  (a) and  $0^\circ$  (b) off the normal to the surface. The spectra were measured at a photon energy of 100 eV.

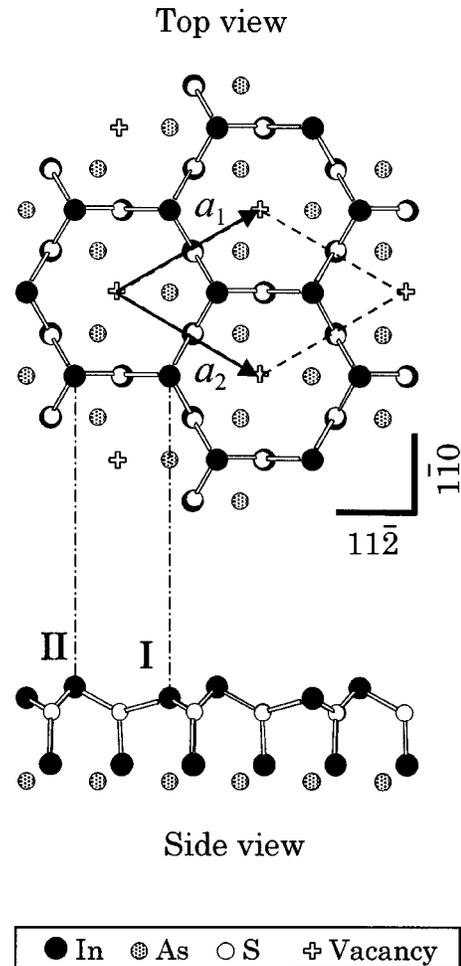


FIG. 8. A model for the InAs(111)A-(2×2)S surface. A broken rhombus corresponds to a 2×2 surface unit cell. The surface unit vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  ( $|\mathbf{a}_1|=|\mathbf{a}_2|=0.86$  nm) are shown. I and II correspond to the In atom located above the As atom in the fourth layer and that above the center of an As triangle in the third layer, respectively.

ing in having an unoccupied dangling bond. The bond length between In and S is assumed to be 0.27 nm, which is close to the sum of the atomic radii of In and S (0.15 and 0.10 nm, respectively<sup>17</sup>). The sulfur coverage for this model is 0.75 ML, which is almost in agreement with the XPS result.<sup>14</sup> The model satisfies the electron counting rule<sup>18</sup> although it contains not only the group-III and -V atoms but also the group-VI atoms, i.e., S. The number of unoccupied dangling bonds in the surface unit cell is two which is less than that (three) for the clean InAs(111)A-(2×2) surface explained by the vacancy-buckling (VB) model.<sup>19</sup> This is consistent with the previous IPES result.<sup>15</sup>

The indium atoms occupy two kinds of the atomic sites, i.e., In(I) and In(II). They correspond to the indium atoms at the sites above the As atoms in the fourth layer and above the center for the triangles of In and As in the third and fourth layers, respectively. The In(I) atoms are located lower than the In(II) atoms by about 0.06 nm, which is consistent with the STM image measured at the positive bias. The sunken In(I) atoms are necessary to explain the *S2s* XPD patterns, as discussed below. The sinking might be derived

from the Coulombic interaction between the In and As atoms in the fourth layer.

For the bulk In atoms in the model, the atoms in the third layer are bonded to one S atom and three As atoms, and those in the fifth layer are bonded to four As atoms. The three main indium components are found for the In  $4d$  spectra in Fig. 6: the one bulk component and two surface components for the  $(2 \times 2)S$  surface. The BEs of the two surface components are shifted higher by +0.58 and +0.30 eV than that of the bulk component. Because S has a larger electronegativity than As, the BE of In  $4d$  at the third layer would be higher than that of the In atoms in the third layer. In addition, since the SCLS of In  $4d$  for the clean InAs(111)A- $(2 \times 2)$  surface,<sup>20</sup> where the In atoms are in a threefold coordination, is about +0.3 eV, the BE shift of the surface indium atoms bonded to sulfur would be larger than +0.3 eV. Therefore, the surface components with the BE shifts of +0.58 and +0.30 eV can be ascribed to the indium atoms at the first and third layers, respectively. Although the atoms at the surface occupy two kinds of sites, the BE difference between In(I) and In(II) would be too small to be distinguished.

As atoms with two kinds of chemical states exist at the fourth layer: the As atom bonded to four In atoms, and that bonded to three In atoms with one occupied dangling bond. The former is located under the In(I) atoms, and the latter around a vacancy of In atoms at the third layer. Because the BEs of the As atoms in threefold and fourfold coordinations cannot be distinguished,<sup>20</sup> one doublet peak appeared in the As  $3d$  spectra shown in Fig. 7.

The honeycomb images clearly observed in Fig. 1 represent a contour of the occupied states at about  $-1.4$  eV below the Fermi level. Surface states localized at  $\sigma$ -type bonds between P and In atoms in the first and second layers for the InP(001)- $(2 \times 4)$  surface,<sup>21</sup> respectively, were found by calculation. In analogy to this result, the images would correspond to surface states localized at the bond between In and S atoms in the first and second layers, respectively, for the proposed model. The detail of the occupied states for the  $(2 \times 2)S$  surface must be investigated by ultraviolet photoelectron spectroscopy and calculation to ensure the above speculation.

In the STM images shown in Figs. 1(a) and 2(a), the defect *A* and bump *B* observed at the positive bias correspond to the defects *A'* and *B'*, respectively, at the negative bias. Since defects *A* and *A'* are observed at the same place, both correspond to a vacancy in the In(II) site. The bump *B* and defect *B'* can be attributed to an indium cluster formed on the In atoms at the first layer. The formation of the indium clusters is suggested by the component *S3* in the In  $4d$  spectra because the SCLS ( $-0.6$  eV) is close to that of the metallic components.<sup>22</sup> However, the other defects observed at the negative bias do not correspond to defects or bumps at positive bias. Further works are necessary for understanding this.

The  $S 2s$  XPD azimuthal patterns were simulated by a single-scattering cluster (SSC) calculation<sup>23</sup> using the model shown in Fig. 8. In the calculation, we take account of three S, five In, and four As atoms included in and below (the fourth layer) the  $2 \times 2$  surface unit cell of the model. Atomic coordinates ( $r_1$ ,  $r_2$ , and  $z$ ) of the above atoms are shown in Table II, where  $r_1$  and  $r_2$  are the lateral components relative

TABLE II. Atomic coordinates ( $r_1, r_2, z$ ) of the structure model shown in Fig. 8. The lateral components  $r_1$  and  $r_2$  refer to the surface unit vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  ( $|\mathbf{a}_1| = |\mathbf{a}_2| = 0.86$  nm), respectively. The vertical component  $z$  is represented in nm.

Atom	$r_1$	$r_2$	$z$ (nm)
In (II)	0.333	0.333	0.00
In (I)	0.667	0.667	-0.06
S	0.016	0.492	-0.13
S	0.492	0.016	-0.13
S	0.492	0.492	-0.13
In	0.000	0.500	-0.40
In	0.500	0.000	-0.40
In	0.500	0.500	-0.40
As	0.167	0.167	-0.49
As	0.167	0.667	-0.49
As	0.667	0.167	-0.49
As	0.667	0.667	-0.49

to the surface unit vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , respectively and  $z$  is the vertical component in nm. The SSC results are superimposed on the experimental patterns in Fig. 4. The unreconstructed (111)A surface structure was used for the calculation. The assumption of the unreconstructed surface is not seriously effective for the As  $3d$  pattern because of the long inelastic mean free path (4.1 nm) of the As  $3d$  photoelectrons excited by a Mg  $K\alpha$  line. The result is also superimposed on the experimental pattern in Fig. 4. The forward-scattered peak of As  $3d$  by the nearest In atoms appears at  $\phi = 60^\circ$  for the simulated As  $3d$  pattern. The strong peaks at  $\phi = 0^\circ$  (at  $\theta = 71^\circ$  and  $78^\circ$ ) and  $60^\circ$  (at  $\theta = 63^\circ$ ) for the simulated  $S 2s$  patterns originate from forward scattering by the nearest In(I) and In(II) atoms, respectively. An *R*-factor analysis<sup>24</sup> is performed for the simulated and experimental patterns for  $S 2s$  and As  $3d$ . The *R* factors obtained for the  $S 2s$  and As  $3d$  patterns are 0.15–0.32 and 0.38, respectively, indicating that both the simulated patterns are in good agreement with the experimental.

Indium vacancies are required in our model. If one indium atom were put on the vacancy site, three unoccupied dangling bonds would exist in the surface unit cell. This is the same number as that on the InAs(111)A- $(2 \times 2)$  surface, which is not consistent with the IPES result.<sup>15</sup> This  $(2 \times 2)S$  model is similar to the VB model,<sup>19</sup> in which the creation of one vacancy in each  $2 \times 2$  cell allows the remaining Ga surface atoms to have a large inward relaxation, resulting in a 2.3-eV reduction in energy. Not only the XPD result but also the total-energy calculation of the surface would be necessary to understand the details of the structure.

The previous XPS result suggested that sulfur is bonded to indium in threefold coordination for the sulfur-adsorbed InAs(111)A and (111)B surfaces.<sup>15</sup> On the other hand, sulfur was adsorbed on gallium at the on-top site for a GaAs(111)A surface, leading to the formation of a  $1 \times 1$  structure.<sup>3</sup> If the sulfur were adsorbed on the on-top site for the InAs(111)A surface, the  $1 \times 1$  structure would be formed. The formation of the different structure, the  $2 \times 2$  structure, which was not found on the other III-V compound semiconductor surfaces, would be due to the preferable

threefold coordination of sulfur with indium on the InAs(111)A surface.

### V. SUMMARY

The structure of the InAs(111)A-(2×2)S surface has been studied by using STM, SRPES, and XPD. Honeycomb-like images with some defects are observed by STM at a bias voltage of  $-1.4$  V. Similar images are also observed at a bias voltage of  $+1.5$  V, although the corners of the hexagon are alternatively depressed in intensity, resulting in a threefold symmetry. The S  $2s$  and As  $3d$  XPD patterns show that most of the sulfur atoms do not occupy sites at the first surface layer, and rarely exchange the fourfold arsenic sites. The three surface and one bulk components are found in the In  $4d$  spectra although one of the surface components

(SCLS:  $-0.6$  eV) cannot be ascribed to the principal constituent of the surface. No surface components are found in the As  $3d$  spectra. Based on STM, SRPES, and XPD results, a probable structure model for the (2×2)S surface is proposed. The SSC calculation of the S  $2s$  XPD patterns is performed using the model. The simulation result is in good agreement with the experimental.

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