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Surface-structure analysis of sulfur-passivated GaAs(111)*A* and GaAs(111)*B* by x-ray standing-wave triangulation

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The positions of sulfur atoms adsorbed on GaAs(111)*A* and GaAs(111)*B* surfaces are determined by x-ray standing-wave (XSW) triangulation studies. On the GaAs(111)*A* surface, which is Ga terminated, sulfur atoms are on top of the first-layer Ga atoms, at the so-called *T* sites. On the GaAs(111)*B* surface, which is As terminated, sulfur atoms exchange with the first-layer As atoms and form bonds with three Ga atoms. These models are consistent with the results of photoemission studies. The S-Ga bond length of 2.41 Å on GaAs(111)*B*, determined from XSW results, is in very good agreement with that derived from the first-principles calculation, suggesting that the substrate surface relaxation is less than the experimental error of 0.04 Å.

I. INTRODUCTION

GaAs electronic device development has been hindered by difficulties in reducing the surface-state density and controlling the Fermi-level position. Since the Na_2S chemical treatment was reported by Sandroff *et al.*,[1] a number of attempts to achieve passivation of GaAs surfaces using sulfide treatment have been made.[2–9] One promising passivation technique is $(NH_4)_2S_x$ treatment, which was reported by Nannichi *et al*[5] The observed effects of this treatment are as follows: (1) enhancement of photoluminescence (PL) intensity,[6] (2) complete removal of oxygen atoms on the surface,[7] (3) clear dependence of the Schottky-barrier height on the work function of the contact metals,[8,9] and (4) improvements in the *C-V* characteristics of metal-insulator-semiconductor (MIS) structures.[6] In order to clarify the causes of these effects, several studies have been made of the $(NH_4)_2S_x$-treated GaAs surfaces. Photoemission spectroscopy studies revealed that both S-Ga and S-As bonds exist on the as-treated surfaces and that thermodynamically stable S-Ga bonds become dominant after annealing at 250–500 °C in a vacuum.[10–12] Although sulfur atoms are found to be bonded to Ga atoms on the $(NH_4)_2S_x$-treated and annealed GaAs surfaces, the three-dimensional adsorption geometry has not yet been determined experimentally.

Ohno and Shiraishi[13,14] suggested the optimal adsorption sites for a monolayer of sulfur atoms on GaAs surfaces by minimizing the total energy, and calculated the electronic structures based on these optimal adsorption configurations. They found that the midgap surface-state density is remarkably reduced and that the Fermi level is shifted toward the valence-band maximum by the formation of stable Ga-S bonds on GaAs(100) and GaAs(111)*A* surfaces. They suggested that the passivation effect can be explained by the actual bonding geometry without introducing any disorder,[15] or any defects,[16] near the surface. In their calculations, in order to determine the optimal structures of sulfur adsorbed on GaAs(111)*A* and GaAs(111)*B*, only two possible 1×1 adsorption geometries, such as exchange and on-top configurations, were considered.[14] However, it has not been discussed whether other adsorption configurations are impossible or not.

While rough surface-normal positions of sulfur atoms on GaAs(111)*A* and GaAs(111)*B* surfaces were studied by soft x-ray standing waves,[17–19] the positions cannot be quantitatively compared with calculated models because there are no good quality data. Furthermore, the inplane positions of sulfur atoms have not yet been investigated at all. The present paper reports the three-dimensional structures of sulfur-passivated GaAs(111)*A* and GaAs(111)*B* surfaces as determined by soft x-ray standing-wave triangulation studies.

The x-ray standing-wave (XSW) technique, first pioneered by Batterman,[20] has been developed into a highly accurate technique of locating the position of particular atomic species in bulk crystal,[21–23] at a crystal surface,[24–29] or at an interface.[30–33] In conventional XSW experiments using hard x rays, the reflection angle is scanned step by step and the secondary-emission yields of particular atomic species are monitored in conjunction with the rocking curve. Recently, a soft x-ray standing-wave technique, which scans the incident photon energy instead of the incident angle, was reported by Ohta *et al.*[34] Since the advantages of this experiment in the back reflection geometry was pointed out by Woodruff *et al.*,[35] several studies utilizing this method have been reported.[36–41] In our S/GaAs(111) system, however, it is impossible to use the back reflection x-ray standing-wave technique because sulfur $K\alpha$ fluorescent x-ray (2.307 keV) cannot be excited by 1.9-keV photons for the normal-incidence GaAs(111) reflection. Therefore, we used the angle-scan soft x-ray standing-wave technique, first reported by Maeyama and co-workers.[42,17] Compared with the conventional hard x-ray standing-wave technique, the angle-scan soft x-ray standing-wave experiment has the following advantages: (1) because of the large intrinsic width of the Bragg reflection (Darwin width), a high mechanical stability of the experimental

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setup is not required; and (2) the large cross sections of soft x-rays for light-element atoms ensure a high emission intensity of the monolayer-order light-element atoms.

From an XSW result, we can only determine the normal distance from the specific bulk-extrapolated reflection planes to the target atoms. Golovchenko *et al.*[43] demonstrate that the three-dimensional position of target atoms can be determined by using plural reflection planes that are not parallel to each other in XSW analysis. Similar triangulation studies have been performed by others.[26,28–30,33]

Here we report the three-dimensional positions of sulfur atoms adsorbed on GaAs(111)A and GaAs(111)B surfaces. We measured the fluorescent x-ray yields excited from both a symmetrical (111) reflection and an asymmetrical $(11\bar{1})$ reflection for the same crystal surfaces. These results enabled us to determine the three-dimensional positions of sulfur atoms relative to the GaAs substrate bulk-extrapolated lattice.

II. EXPERIMENT

The substrates were n-type GaAs(111)A and GaAs(111)B wafers. The wafers were treated with a $(NH_4)_2S_x$, $x=3$ solution for 1 h at 60 °C. These sulfur-treated samples were then annealed at about 300 °C in a vacuum for 10 min. It has been found that there are S-Ga bonds on the annealed surface and that 1×1 low-energy electron-diffraction (LEED) and reflection high-energy electron-diffraction (RHEED) patterns are obtained for both (111)A and (111)B surfaces.[10] These samples were next transferred to an XSW analysis chamber without being exposed to the air.

Soft x-ray standing-wave experiments were carried out at the NTT beamline 1A of the Photon Factor at the National Laboratory for High Energy Physics. Synchrotron radiation emitted from a normal bending magnet is first reflected by a front mirror and monochromatized by InSb(111) double crystals and then reflected by a rear mirror.[44] The photon energy was fixed at 2.47 keV and the incident angle was scanned step by step near the Bragg reflection of the GaAs(111) substrate. The intensities of the Bragg reflection were monitored by photocurrents measured with a Cu plate, and the incident beam was measured with a semitransparent Au grid. Sulfur $K\alpha$ fluorescent x rays were collected by a highly pure Si detector. In order to determine the three-dimensional positions of the sulfur atoms, we have studied both the symmetrical (111) reflection and the asymmetrical $(11\bar{1})$ reflection for each sample. When the (111) XSW experiment was completed, χ and ϕ axes of vacuum goniometer[45] were tuned to set up the $(11\bar{1})$ experiment.

III. RESULTS AND DISCUSSION

It has been reported that the signal to background (SB) ratio of the fluorescent x-ray yield excited by soft x rays is higher than that of the Auger-electron yield.[36,38] Figure 1 shows the fluorescent x-ray spectra for S/GaAs(111) excited by synchrotron radiation soft x rays. As can be seen, a sulfur $K\alpha$ fluorescent x-ray peak is clearly separated from other peaks, such as Ga L and As L, because of the high-energy resolution of the highly pure Si detector. In previous work, Ga L from As L could not be separated by the Si (Li) detector. Furthermore, the detector was not in the polarized direction of the incident synchrotron radiation x rays. Thus the Compton and thermal diffuse scattering signals were observed and high background in the fluorescent x-ray spectra were formed by these scattering signals. Furthermore, the angular-dependent detector's dead time, which was caused by these scattering signals, might affect the measured fluorescent x-ray yields. In this study, the influence of these scattering signals can be eliminated by collecting the fluorescent x-ray yields from the polarized direction.[46] By this improvement an angular-dependent fluctuation of the detector's dead time can be suppressed, and reliable measurement of the angular-dependent sulfur $K\alpha$ fluorescent x-ray yields can be realized.

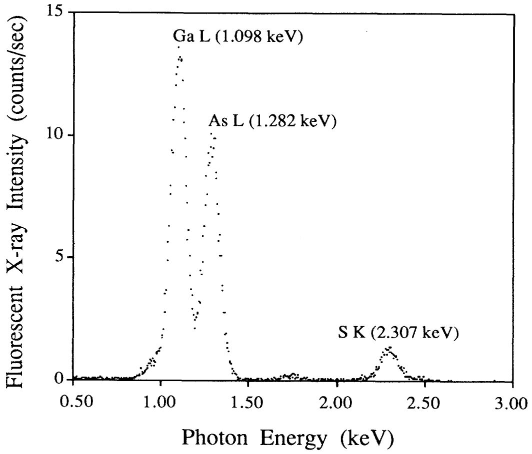


FIG. 1. Fluorescent x-ray spectra from sulfur on a GaAs(111)B surface which was excited by photons of 2.47 keV, collected with a highly pure Si detector in the polarized direction.

Figure 2 shows the angular dependence of the fluorescent x-ray yields for Ga L and As L collected by a highly pure Si detector, and the reflectivity of the (111) Bragg reflection from a GaAs(111)B crystal using 2.47-keV soft x rays. The angular width of the intrinsic Bragg reflection is nearly proportional to $\lambda^2/\sin(2\theta_B)$, where λ is the wavelength and θ_B the Bragg angle. For example, with symmetric Bragg case GaAs(111) reflection, the angular width of 79 arc sec for 2.47-keV soft x-rays is about ten times larger than the 7.3 arc sec for 17.4-keV hard x rays. The observed Bragg reflection width in Fig. 2, which is about 100 arc sec, is not far from the intrinsic width. To measure the fluorescent x-ray yields, a highly pure Si detector was located at a glancing angle with respect to the (111) crystal surface without using any slits in front of the fluorescent x-ray detector.

We also found that the extinction effect for bulk fluorescent x rays[47] was reduced. This can be attributed to the following reasons. The larger absorption coefficient of the incident soft x rays than of the hard x rays makes the penetration depth of the incident beam very shallow

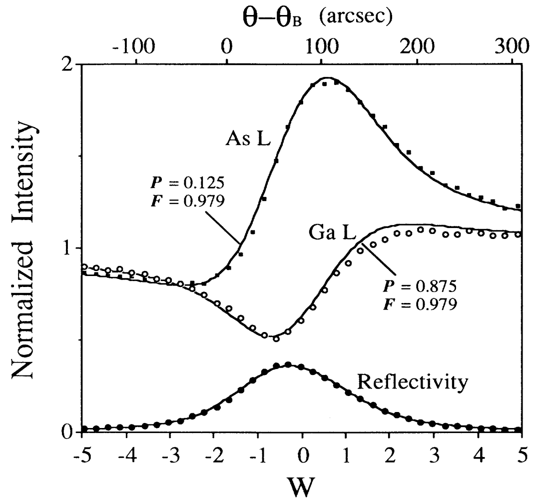


FIG. 2. Angular dependence of the fluorescent x-ray yield curves for Ga *L* (open circles) and As *L* (solid squares), and the reflectivity (solid circles) of the (111) reflection from a GaAs(111)*B* crystal using incident synchrotron radiation soft x rays of 2.47 keV. *W* is the normalized angle. Lines are calculated curves. The detector was located at a grazing angle with respect to the (111) crystal surface.

even under the off-Bragg condition. Furthermore, the large absorption coefficients of the low-energy bulk fluorescent x rays make the escape depth of emitted fluorescent x rays shallow.

The angular-dependent fluorescent x-ray yield $Y_{(\theta)}$ is given by

$$Y_{(\theta)}=1+R_{(\theta)}+2F\sqrt{R_{(\theta)}}\cos(2\pi P-\delta_{(\theta)}) , \tag{1}$$

where $R_{(\theta)}$ is the intrinsic reflectivity and $\delta_{(\theta)}$ the phase between the two plane waves which form the interference field. $R_{(\theta)}$ and $\delta_{(\theta)}$ can be computed as a function of incident angle θ for the GaAs(111) reflection.[32,46,48,49] The two parameters *P* and *F*, that are determined in an XSW experiment, are the coherent position and the coherent fraction, respectively. These parameters contain structural information on target atoms. The coherent position *P* gives the position of target atoms with respect to the specific bulk-extrapolated reflection planes. The coherent fraction *F* includes both the Debye-Waller factor and the fraction of the atoms at the actual lattice sites defined by the coherent position *P*.

In our analysis, the anomalous atomic scattering factors reported by Henke *et al.*[50] were used. On the other hand 0.979, which is simply calculated from $B=0.91$ Å^2,[51,52] was used for room-temperature Debye-Waller factors of the Ga and As atoms in the GaAs(111) reflection.[46,48] $R_{(\theta)}$ and $Y_{(\theta)}$ were convoluted by instrumental resolution. In this calculation, the instrumental resolution was simulated as 60% Gaussian plus 40% Lorentzian, where full width at half maximum (FWHM) for both was 75 arc sec. The two upper solid lines in Fig. 2 are profiles calculated with *P* and *F* values of 0.875 and 0.979 for Ga and 0.125 and 0.979 for As. They agree well with the experimental Ga *L* and As *L* fluorescent x-ray profiles. The correct instrumental resolution of the soft x-ray beam can be estimated, suggesting that the resolution cannot be estimated using only Gaussian profiles.[53]

In order to estimate the accuracy of atomic positions determined by this analysis, Ga *L* and As *L* yields were fitted without any assumption. The best fits for Ga *L* and As *L* yields were obtained for *P* and *F* values of 0.864(1) and 0.957(4) and 0.113(1) and 0.946(8), respectively. Therefore, atomic positions determined by the analysis are reliable within an error of 0.04 Å which can be estimated by the difference between 0.875 and 0.864(1) for Ga, and by the difference between 0.125 and 0.113(1) for As. Furthermore, it must be noted that statistical errors obtained by standard deviations of *P* values are smaller than the analytical error of about 0.04 Å.

A. S/GaAs(111)*A*

Figure 3(a) shows the soft x-ray standing-wave result for the (111) reflection. A P_{111} of 0.791(3) and an F_{111} of 0.86(2) were obtained. The scattering of data points in this figure is much smaller than for our previous work.[18] The background intensity in the fluorescent x-ray spectra was eliminated by the improvement of the experimental setup; we could collect sulfur emission intensities in the high SB ratio. Though this sample was treated by the wet method and annealed in a vacuum, an appreciably high F_{111} of 0.86 was obtained. This indicates that a well-ordered GaAs(111)*A* surface can be obtained by using the $(NH_4)_2S_x$ treatment. On the other hand, Fig. 3(b) shows the result of the $(11\bar{1})$ reflection, where a $P_{11\bar{1}}$ of 1.00(1) and an $F_{11\bar{1}}$ of 0.65(2) were obtained. The $F_{11\bar{1}}$ of 0.65 is lower than the F_{111} of 0.86. This may indicate that the in-plane position of sulfur atoms is less ordered than the surface-normal direction. It is thought that there is an ambiguity in the experimental $P_{11\bar{1}}$ value, because the rocking curve of $(11\bar{1})$ reflection is slightly broad. This means that error of the $P_{11\bar{1}}$ value is much larger than 0.01, which was estimated only by a standard deviation. However, we can choose the most probable model by this result.

Figure 4 shows three possible adsorption sites of sulfur

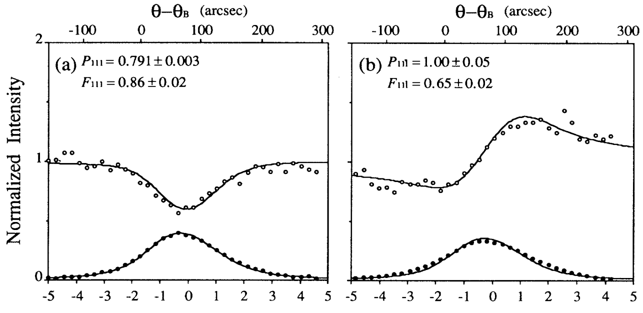


FIG. 3. Results of the soft x-ray standing-wave measurements on S/GaAs(111)*A*: (a) (111) reflection, and (b) $(11\bar{1})$ reflection. The solid circles are the rocking-curve data points. The open circles are the sulfur $K\alpha$ fluorescent x-ray yield data points. The solid curves are the theoretical fits to the data.

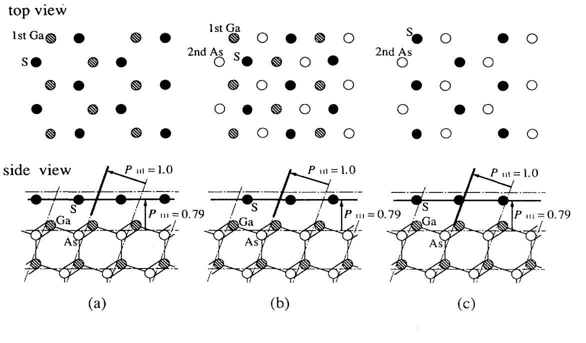


FIG. 4. Schematic showing the position of the sulfur atoms (solid circles) with respect to the GaAs(111)*A* substrate from both top and side views. The surface-normal direction is defined as [111]. The open and hatched circles are As and Ga atoms, respectively. (a) *T*4 site, which is fourfold coordinated on top of the second-layer atoms; (b) *H*3 site, which is threefold coordinated on top of the fourth-layer atoms; and (c) *T* site, which is onefold coordinated on top of the first-layer atoms.

atoms on GaAs(111)*A*, referred to as the *T*4, *H*3, and *T* sites. They are based on simply considering the experimental surface-normal coherent position P_{111} of 0.791. Each model in Fig. 4 is a simple 1×1 structure with the S-Ga bonds dominant. Two lines determined by two types of XSW results cross each other between the H3 and *T* sites as shown in Fig. 4. The experimental $P_{11\bar{1}}$ value is closer to the ideal one for the *T*-site model than those for other models as shown in Table I, but they do not agree well. It is known that the coherent fraction *F* should include the Debye-Waller factor and the fraction of the atoms that are located at the actual lattice sites. In the XSW study of CaF_2 on Si(111) reported by Zegenhagen and Patel,[33] who used the XSW results of (111) and (220) reflections, it was concluded that Ca atoms are located at both the *H*3 and *T*4 sites, which are at the same surface-normal position. This is possible because *T*4 and *H*3 are highly symmetrical adsorption sites. In our case, however, it cannot be thought that sulfur atoms at the *H*3 and *T* sites are at the same surface-normal position because the *H*3 and *T* sites are not highly symmetrical sites. Furthermore, the high surface-normal coherent fraction F_{111} of 0.86 indicates that sulfur atoms are not located at both the *H*3 and *T* sites. We therefore conclude that sulfur atoms are on top of the first-layer Ga atoms on the GaAs(111)*A* surface as shown in Fig. 4(c). The *T*-site model is in good agreement with the calculated "on-top configuration" reported by Ohno.[14] The S-Ga bond length of 2.17 Å, which is calculated from the experimental P_{111} values by assuming no relaxation of the substrate lattice, is also very close to the calculated bond length of 2.11 Å when the total energy is minimized.[14] The bond length of 2.17 Å, which is slightly shorter than the 2.33 Å for GaS,[54] implies that the S-Ga bond has a covalent sp^3 character in this structure. Our results verified that the structure of a $(NH_4)_2S_x$-treated and annealed GaAs(111)*A* surface is the *T*-site model shown in Fig. 4(c), which is the same model used for calculating the surface electronic structure of S/GaAs(111)*A*.[14]

TABLE I. Experimental $P_{11\bar{1}}$ value compared with the ideal $P_{11\bar{1}}$ values, which are calculated from the experimental P_{111} of 0.791, for each model shown in Fig. 4. The S-Ga bond length of the *T*-site model was calculated from the experimental P_{111} of 0.791 assuming no relaxation of the substrate lattice. Theoretical value of the "on-top configuration" reported by Ohno are also shown.

	P_{111}	$P_{11\bar{1}}$	S-Ga (Å)
Experimental result	0.791(3)	1.00(>1)	
*T*4-site model [Fig. 4(a)]	0.791	0.430	
*H*3-site model [Fig. 4(b)]	0.791	0.764	
T-site model [Fig. 4(c)]	0.791	1.097	2.17
Theory (*T*-site model)	0.77	1.09	2.11

The experimental P_{111} value obtained from the XSW result gives the normal distance from the specific bulk-extrapolated (111) reflection planes to sulfur atoms. Patel *et al.*[36] and Yokoyama *et al.*[38] reported that the surface relaxation can be studied by using XSW results, and the bond lengths determined by surface extended x-ray-absorption fine structure. Unfortunately, the S-Ga bond lengths on the GaAs(111) surface have not been determined by another experimental result. Although we assumed no relaxation of the substrate lattice to obtain the S-Ga bond length of 2.17 Å, this value agrees with that reported by Ohno[14] within a 10^{-2}-Å order. This may be attributed to little relaxation of the first-layer Ga atoms at this surface.

B. S/GaAs(111)*B*

Figure 5(a) shows the soft x-ray standing-wave result for the (111) reflection. The scattering of data points is also much better than in our previous work.[17,18] A P_{111} of 0.089(4) and an F_{111} of 0.81(2) were obtained. The F_{111} of 0.81 for the (111)*B* surface is slightly smaller than the 0.86 for the (111)*A* surface. This may be due to the more than 1-monolayer (ML) sulfur coverage, where sulfur

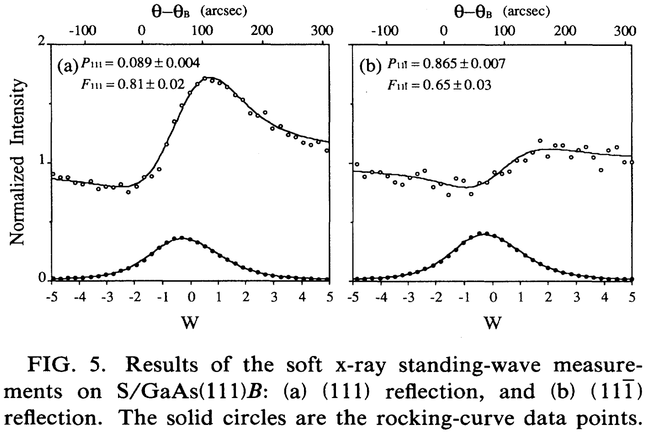
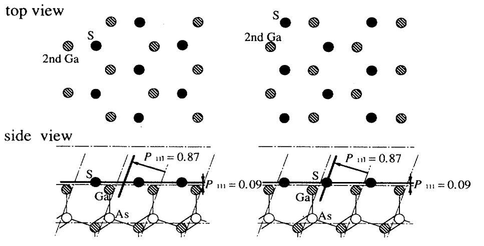


FIG. 5. Results of the soft x-ray standing-wave measurements on S/GaAs(111)*B*: (a) (111) reflection, and (b) $(11\bar{1})$ reflection. The solid circles are the rocking-curve data points. The open circles are the sulfur *Kα* fluorescent x-ray yield data points. The solid curves are the theoretical fits to the data.

TABLE II. Experimental $P_{11\bar{1}}$ value compared with the ideal $P_{11\bar{1}}$ values, which are calculated from the experimental P_{111} of 0.089 for each model shown in Fig. 6. The S-Ga bond length of the exchange model was calculated from the experimental P_{111} of 0.089, assuming no relaxation of the substrate lattice. Theoretical values of the "exchange configuration" reported by Ohno are also shown.

	P_{111}	$P_{11\bar{1}}$	S-Ga (Å)
Experimental result	0.089(4)	0.865(7)	
S-site model [Fig. 4(a)]	0.089	0.530	
E-site model [Fig. 4(b)]	0.089	0.863	2.41
Theory (*E*-site model)	0.09	0.86	2.41



(a) (b)

FIG. 6. Schematic showing the position of the sulfur atoms (solid circles) with respect to the GaAs(111)*B* substrate from both top and side views. Here, the surface-normal direction is defined as [111], which is opposite to the general definition. The open and hatched circles are As and Ga atoms, respectively. (a) Stacking fault site. (b) Exchange site.

atoms may exist at the third layer As atom site. In particular, the sulfur $K\alpha$ fluorescent x-ray intensity of the (111)*B* sample is slightly larger than that of the (111)*A* sample. In such a case, the position of first-layer sulfur does not become completely equivalent to that of the third layer, and this results in a smaller coherent fraction *F*. Figure 5(b) shows the soft x-ray standing-wave result for the $(11\bar{1})$ reflection. A $P_{11\bar{1}}$ of 0.865(7) and an $F_{11\bar{1}}$ of 0.65(3) were obtained. The $F_{11\bar{1}}$ of 0.65 is lower than the F_{111} of 0.81 for the (111)*B* surface as with the (111)*A* surface. This also indicates that the in-plane position of the sulfur atom is less ordered than the surface-normal direction.

The surface-normal position determined by P_{111} of 0.089 is equivalent to that of 1.089. However, the S-Ga bond length expected from the P_{111} of 1.089 is too long in each model. Therefore, the two structure models shown in Fig. 5 can only be considered from the experimental surface-normal coherent position P_{111} of 0.089. In both models in Fig. 5, the position is very close to the first-layer As atoms, so As atoms must be missing from the first layer. Two lines determined by two types of XSW results cross each other just at the exchange site. In particular, the experimental $P_{11\bar{1}}$ of 0.865(7) agrees well with the ideal $P_{11\bar{1}}$ for the exchange model of 0.863 shown in Table II. Therefore, sulfur atoms exchange with the first-layer As atoms and each sulfur atom forms bonds with three Ga atoms as shown in Fig. 6(b). This structure model is in agreement with the "exchange configuration" reported by Ohno.[14] Furthermore, the S-Ga bond length of 2.41 Å, which is calculated from the experimental P_{111} of 0.089 by assuming no relaxation of the substrate lattice, is slightly longer than the 2.33 Å for GaS,[54] and agrees well with the bond length of 2.41 Å calculated by Ohno.[14] This may also be attributed to a small relaxation of the first-layer Ga atoms at this surface. Therefore, the structure of $(NH_4)_2S_x$-treated and -annealed GaAs(111)*B* surface is found to be the exchange model shown in Fig. 4(c), which is the same as that used for calculating the surface electronic structure of S/GaAs(111)*B*.[14]

IV. CONCLUSION

The surface structures of sulfur-passivated GaAs(111)*A* and GaAs(111)*B* are determined by the soft x-ray standing-wave triangulation. On the GaAs(111)*A* surface, sulfur atoms are on top of the first-layer Ga atoms. On the GaAs(111)*B* surface, the sulfur atoms exchange with the first-layer As atoms forming bonds with three Ga atoms. The S-Ga bond lengths determined from XSW results agree well with those derived from first-principles calculation. Therefore, it can be thought that there is little relaxation at the surface.

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