

# Charge transfer and structure of K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface studied by reflection high-energy positron diffraction

Y. Fukaya,\* I. Mochizuki, and A. Kawasuso

*Advanced Science Research Center, Japan Atomic Energy Agency, 1233 Watanuki, Takasaki, Gunma 370-1292, Japan*

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The atomic coordinates and charge transfer of the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface were investigated using reflection high-energy positron diffraction (RHEPD). Upon the adsorption of K onto the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface, the position of the 111 Bragg reflection is shifted to a lower angle, thus suggesting that a change in the inner potential arises from the charge transfer of  $1.0e^-$  per K atom to the surface. From RHEPD rocking curves recorded at 113 K, we determined that the top K atoms and the Si adatoms are adsorbed 2.96 and 2.51 Å from the first Si layer, respectively. The Si adatoms are significantly displaced upward compared to that found for the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface. Furthermore, we found that the K atoms are adsorbed between the  $H_3$  and  $T'_4$  sites. These are consistent with the recent theoretical prediction that the Si adatoms are upwardly displaced and the K atoms form a trimer structure in the  $2\sqrt{3} \times 2\sqrt{3}$  unit cell at low temperature [*Phys. Rev. Lett.* **107**, 187603 (2011)], although the flat model where all the Si adatoms have the same height is also acceptable in the rocking curve analyses. However, at room temperature, which is above the surface phase-transition temperature for  $2\sqrt{3} \times 2\sqrt{3}$  to  $\sqrt{3} \times \sqrt{3}$ , the K atoms are randomly located in the  $2\sqrt{3} \times 2\sqrt{3}$  unit cell. This phase transition is accompanied by the disordering of K atoms.

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## I. INTRODUCTION

The highly B-doped Si(111) surface possesses a  $\sqrt{3} \times \sqrt{3}$  structure with the B atoms located at the  $S_5$  site (see Fig. 1).<sup>1-3</sup> When the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface is saturated by K atoms at room temperature, the K/Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface is formed. This surface is known as a Mott insulator.<sup>4</sup> The electronic structure of the K/Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface has been extensively investigated using angle-resolved photoemission spectroscopy. However, the atomic configuration of the K/Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface is still under debate. In particular, the atomic positions of the K atoms have yet to be confirmed experimentally.<sup>5</sup> Furthermore, it is argued that the saturation coverage ( $\rho$ ) of the K atoms is a third or a half of a monolayer (ML, 1 ML =  $7.83 \times 10^{14}$  cm<sup>-2</sup>).<sup>4,6</sup>

Recently, it has been reported that the K/Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface undergoes a phase transition from the  $\sqrt{3} \times \sqrt{3}$  to  $2\sqrt{3} \times 2\sqrt{3}$  structure at temperatures below 270 K.<sup>7</sup> From photoemission spectroscopy, the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface is considered to be a bipolaronic insulator.<sup>7,8</sup> However, the atomic configuration of the  $2\sqrt{3} \times 2\sqrt{3}$  structure is also unknown experimentally.<sup>9</sup> From a structural point of view, there are two possible atomic configurations for the  $2\sqrt{3} \times 2\sqrt{3}$  structures with the bipolaron. One is the “one-up and three-down” (1U3D) model, where one Si adatom is located at a relatively higher position than the other three Si adatoms in the unit cell. The other is the “three-up and one-down” (3U1D) model, where one adatom is located at a relatively lower position than the other three atoms in the unit cell.

Reflection high-energy positron diffraction (RHEPD) is a sensitive tool for the topmost surface because of the total reflection. Since the positron has a positive charge and hence the crystal potential acts as a potential barrier, the total reflection occurs at grazing incidence.<sup>10,11</sup> In this study, we investigated the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface structures by RHEPD at both above and below the phase-transition temperature. Shown are the atomic positions and disordering of

the K atoms that result from the  $\sqrt{3} \times \sqrt{3}$ - $2\sqrt{3} \times 2\sqrt{3}$  phase transition. Furthermore, we estimate the amount of charge transfer from the K to Si atoms.

## II. EXPERIMENT

Substrates ( $10 \times 5 \times 0.5$  mm<sup>3</sup>) were cut from a highly B-doped, mirror-polished Si(111) wafer.<sup>12</sup> These were flashed a few times at 1470 K in an ultrahigh vacuum (UHV) chamber with a base pressure of less than  $2 \times 10^{-8}$  Pa. After annealing at 1170 K, a well-ordered  $\sqrt{3} \times \sqrt{3}$  structure was formed.<sup>13</sup> Subsequently, the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface was saturated by the K atoms at room temperature.

A well-collimated and highly parallel positron beam of energy 10 keV was irradiated onto the sample surface at grazing incidence. The diffraction patterns were observed using a microchannel plate with a phosphor screen and a charge-coupled-device camera. By rotating the sample, the glancing angle ( $\theta$ ) of the incident positron beam was varied from 0.3° to 6.0° in steps of 0.1°. Details of the positron beam apparatus are described elsewhere.<sup>14</sup>

## III. RESULTS AND DISCUSSION

Figure 2 shows the RHEPD rocking curves for the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface at 295 K. The incident azimuth of the positron beam is 7.5° away from the [112] direction (one-beam condition<sup>15</sup>). Under this condition, the rocking curve mainly depends upon the atomic positions that are perpendicular to the surface. In the total reflection region ( $\theta < 2.0^\circ$ ), the specular intensity is high and a small dip in the curve is clearly observed at 1.8°. In addition, distinct peaks for the 111 and 222 Bragg reflections and weak 333 and 444 Bragg reflection peaks are clearly visible.

In order to verify the atomic configuration of the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B substrate, we calculated the RHEPD intensities

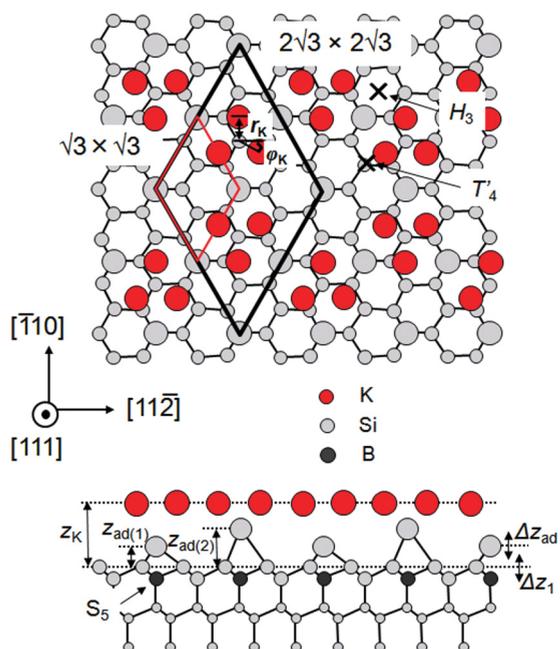


FIG. 1. (Color online) Schematic drawing of the Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface. Red, gray, and black circles indicate K, Si, and B atoms, respectively. The  $2\sqrt{3} \times 2\sqrt{3}$  and  $\sqrt{3} \times \sqrt{3}$  unit cells are indicated by the black and red lines, respectively.  $r_K$  and  $\varphi_K$  denote the polar coordinates of the K atoms.

on the basis of the dynamical diffraction theory.<sup>16</sup> In the calculations, the thermal vibrational amplitude of the Si and B atoms were assumed to be  $7.84 \times 10^{-2}$  Å.<sup>17</sup> The adsorption potentials resulting from the electronic excitations were assumed to be a fitting parameter for the surface layer and 1.70 eV for the bulk layer.<sup>18</sup> Two heights of Si adatoms ( $z_{ad}$ ) and the first layer ( $z_1$ ) of Si atoms were varied so as to minimize the difference between the experimental and calculated curves. The goodness of fit was judged via the reliability ( $R$ ) factor.<sup>19</sup> The solid line in Fig. 2 represents the calculated rocking curve for the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface using the optimized atomic configuration and it is shown that the calculated curve is in good agreement with the measured curve. In the fitting procedure, with respect to the ideal Si bulk positions, we obtained  $\Delta z_{ad} = +0.24 \pm 0.10$  Å and  $\Delta z_1 = -0.46 \pm 0.06$  Å (see Fig. 1). The structure parameters are summarized in Table I. The atomic displacements obtained here are in good agreement with those previously obtained by experiment and calculation.<sup>3,20-22</sup>

Figure 3(a) shows the RHEPD rocking curves for the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface at 113 K under the one-

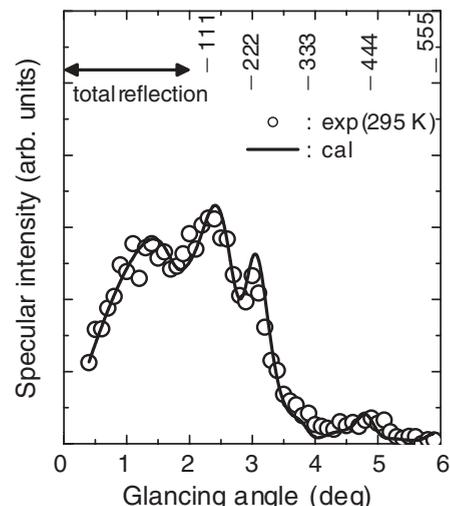


FIG. 2. RHEPD rocking curves of the specular spot from the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface under the one-beam condition. The incident azimuth of the positron beam is  $7.5^\circ$  with respect to the  $[11\bar{2}]$  direction. The open circles denote the experimental curve at 295 K. The solid line indicates the curve calculated using the heights of the optimum adatom and first Si layer. The acceleration voltage of the incident positron beam is 10 kV. The critical angle of the total reflection is estimated to be  $2.0^\circ$  via Snell's equation.

beam condition. In the rocking curve for the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface, we observe intense 111 and 222 Bragg reflection peaks and weak 333 and 444 Bragg peaks. In the total reflection region, the dip in the curve that results from the adsorption of K atoms appears at  $1.2^\circ$ . Upon deposition of the K atoms, the position of the 111 Bragg peak is dramatically shifted to a lower angle compared to that found for the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface (Fig. 2). This suggests that there is a reduction in the inner potential due to the adsorption of K atoms.

We first estimate the change in the mean inner potential from the shifts of the Bragg peaks in the RHEPD rocking curves. The peak positions in the rocking curve obey the Bragg equation. In the crystal, the glancing angles that satisfy the Bragg condition are varied due to the refraction. The refractive index can be expressed using Snell's equation as  $\cos\theta_c/\cos\theta_v = \sqrt{E/(E + eV_0)}$ , where  $\theta_v$  and  $\theta_c$  denote the glancing angles of the incident positron before and after refraction, respectively, and  $V_0$  and  $E$  are the mean inner potential and accelerating energy of the incident positron, respectively.<sup>10</sup> Thus the peak position is finally determined by the mean inner potential ( $V_0$ ). In order to estimate the mean inner potential of the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface, we

TABLE I. Structure parameters for the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B and the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surfaces.

	$r_K$	$\varphi_K$	$z_K$	$z_{ad}$	
				$z_{ad(1)} \rho_{Si} = 1/12$ ML	$z_{ad(2)} \rho_{Si} = 3/12$ ML
Si(111)- $\sqrt{3} \times \sqrt{3}$ -B				$1.49 \pm 0.10$ Å	
K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B ( $\rho_K = 1/2$ ML)	$2.31 \pm 0.37$ Å	$43.4 \pm 7.8^\circ$	$2.96 \pm 0.10$ Å	$2.51 \pm 0.83$ Å	$2.51 \pm 0.23$ Å
K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B ( $\rho_K = 1/3$ ML)			2.20 Å	1.15 Å	1.15 Å

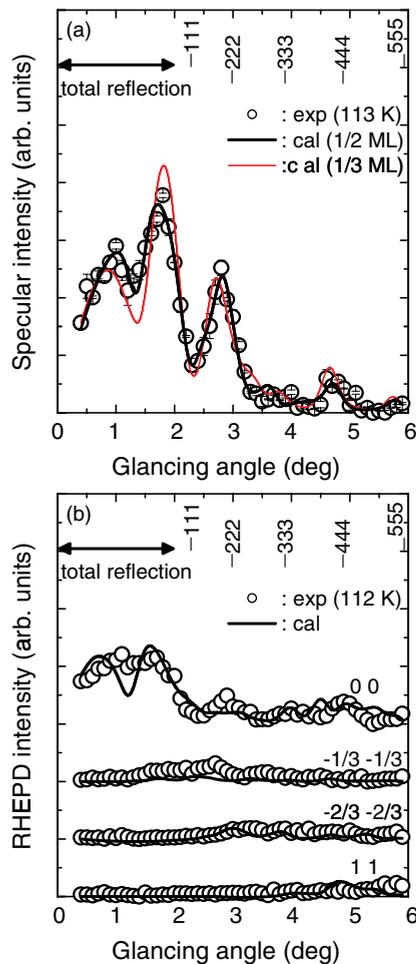


FIG. 3. (Color online) (a) RHEPD rocking curves of specular spots for the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface at 113 K under the one-beam condition. (b) RHEPD rocking curves of the (0 0),  $(-1/3 -1/3)$ ,  $(-2/3 -2/3)$ , and (1 1) spots from the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface at 112 K along the  $[11\bar{2}]$  direction. The circles indicate the experimental curves. In (a), the black and red lines denote the calculated curves using the optimum heights of K atoms and the Si adatoms at  $\rho_K = 1/2$  ML and  $\rho_K = 1/3$  ML, respectively. In (b), the solid lines show the calculated curves when it is assumed that the surface structure is composed of the K trimers.

varied  $V_0$  so as to reproduce the experimental peak positions. As a result of finding the minimum in  $R$ , we determined  $V_0 = 8.6 \pm 0.5$  eV for the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface. Therefore  $V_0$  changes from 12 to 8.6 eV as a result of the K atom deposition.

The change in the mean inner potential corresponds to the formation of the surface dipole. The change in the potential due to the dipole formation is given as  $\Delta V_0 = end/\epsilon_0$ , where  $n$ ,  $d$  and  $\epsilon_0$  are the number density of K ions, the distance between charges, and the permittivity, respectively. For the adsorption position of the K atoms ( $d = 0.46$  Å), comparison of their number density to that of the K atoms in the unit cell ( $n = 0.041$  Å $^{-2}$ , cf.  $0.039$  Å $^{-2}$ ) means that we can estimate the amount of charge transfer from the K to Si atom as  $1.0e^-$  per K atom at 113 K.

In considering  $V_0 = 8.6$  eV and the theoretical prediction for the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface with  $\rho_K = 1/2$  ML,<sup>6,9</sup> we optimized the height ( $z_K$ ) of the K atoms and two independent heights ( $z_{ad(1)}$  with  $\rho_{Si} = 1/12$  ML and  $z_{ad(2)}$  with  $\rho_{Si} = 3/12$  ML) for the Si adatoms by means of the  $R$  factor so as to minimize the difference between the measured and calculated curves. For the calculations, the thermal vibrational amplitudes of the K atoms were assumed to be  $2.16 \times 10^{-1}$  Å.<sup>17</sup> As shown by the black line in Fig. 3(a), the calculated curve is in good agreement with experiment if we assume that the positions of the K atoms and the Si adatoms are  $z_K = 2.96 \pm 0.10$  Å,  $z_{ad(1)} = 2.51 \pm 0.83$  Å, and  $z_{ad(2)} = 2.51 \pm 0.23$  Å from the first Si layer, respectively (see also Table I). As a result, we found that the K atoms and the Si adatoms are farther away from the first Si layer. In considering the large error bar of  $z_{ad(1)}$ , both the 1U3D and 3U1D models are acceptable as well as the flat model where all the Si adatoms have the same height. In the case of the 3U1D model, the averaged height of the Si adatoms is smaller than 2.51 Å. This indicates that the amount of charge transfer from the K to Si atom is less than  $1.0e^-$  per K atom. In the case of the 1U3D model, the amount of charge transfer is larger than  $1.0e^-$  per K atom. However, the charge transfer larger than  $1.0e^-$  per K atom is not physically acceptable. Thus, considering the large error bar of  $z_{ad(1)}$  due to the lower coverage, the structure model determined in this study is consistent with the flat model and the 3U1D model proposed by the recent theoretical calculations.<sup>9</sup> Since the saturation coverage of the K atoms has not been confirmed yet, we also calculated the rocking curves taking into account the structure model with  $\rho_K = 1/3$  ML.<sup>4,5</sup> As shown by the red line in Fig. 3(a), the calculated curve using  $\rho_K = 1/3$  ML is inconsistent with the experiment, as compared to that for  $\rho_K = 1/2$  ML. Thus the saturation coverage of  $\rho_K = 1/2$  ML is more plausible. In a previous theoretical study,<sup>5</sup>  $H_3$  or  $T'_4$  are suggested as possible adsorption sites. The positions of the K atoms are estimated to be 2.36 and 2.49 Å for the  $H_3$  and  $T'_4$  sites, respectively.<sup>5</sup> The position of the K atoms determined in this study is higher than these values, thus implying that the adsorption site of the K atoms is shifted from the  $H_3$  or  $T'_4$  sites.

To confirm the adsorption site of the K atoms, we measured the rocking curves along the  $[11\bar{2}]$  direction. The open circles in Fig. 3(b) show the measured rocking curves for the K/Si(111)- $2\sqrt{3} \times 2\sqrt{3}$ -B surface along the  $[11\bar{2}]$  direction at 112 K. On the basis of the theoretical results,<sup>9</sup> we calculated the RHEPD rocking curves assuming that the K atoms form a trimer structure on the Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface. Then, we optimized the length ( $r_K$ ) and the rotation angle ( $\phi_K$ ) of the K trimer so as to minimize the difference between the measured and calculated curves (see Fig. 1). The solid lines in Fig. 3(b) show the calculated rocking curves for the K/Si(111)- $\sqrt{3} \times \sqrt{3}$ -B surface using the optimum length ( $r_K = 2.31$  Å) and rotation angle ( $\phi_K = 43.4^\circ$ ) for the K trimer (see also Table I). The measured curves can be reproduced by the calculated curves using the trimer model. The bond length between the K atoms determined here is estimated to be 4.00 Å, which is in good agreement with the average between the metallic (4.70 Å) and ionic bondings (2.74–3.28 Å). Therefore the adsorption site of the K atoms corresponds to an intermediate position between the  $H_3$  and  $T'_4$  sites. Recent

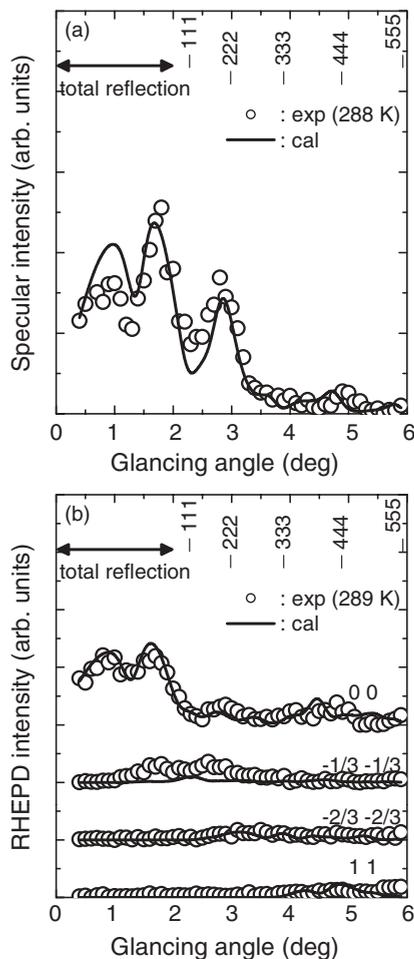


FIG. 4. (a) RHEPD rocking curves of specular spots from the  $\text{K/Si(111)-}\sqrt{3} \times \sqrt{3}$ -B surfaces at 288 K under the one-beam condition. (b) RHEPD rocking curves of the (0 0),  $(-1/3 -1/3)$ ,  $(-2/3 -2/3)$ , and (1 1) spots from the  $\text{K/Si(111)-}\sqrt{3} \times \sqrt{3}$ -B surface at 289 K along the  $[11\bar{2}]$  direction. The circles indicate the experimental curves. In (a), the solid line denotes the calculated curve using the optimum heights determined at 113 K. In (b), the solid lines show the calculated curves when the K atoms are assumed to be randomly situated at the intermediate positions between the  $H_3$  and  $T'_4$  sites.

theoretical studies suggested that the K atoms were located between the  $H_3$  and  $T'_4$  sites.<sup>9</sup> The present model is consistent with the theoretical calculations.

Figure 4(a) shows the RHEPD rocking curves for the  $\text{K/Si(111)-}\sqrt{3} \times \sqrt{3}$ -B surface at 288 K under the one-beam condition. The shape of the curve is not changed from that observed for the  $\text{K/Si(111)-}2\sqrt{3} \times 2\sqrt{3}$ -B surface at 113 K [Fig. 3(a)], which suggests that there are no displacements of the K atoms and the Si adatoms due to the phase transition from the  $2\sqrt{3} \times 2\sqrt{3}$  to  $\sqrt{3} \times \sqrt{3}$  structure. The position of the 111 Bragg peak is nearly the same as that for the  $\text{K/Si(111)-}2\sqrt{3} \times 2\sqrt{3}$ -B surface. This indicates that the mean inner potential is almost unchanged upon the phase transition.

The solid line in Fig. 4(a) shows the calculated rocking curve for the  $\text{K/Si(111)-}\sqrt{3} \times \sqrt{3}$ -B surface using the optimum heights of the K atoms and the Si adatoms determined

at 113 K. The calculations are capable of reproducing the experimental data. To verify the adsorption site of the K atoms for the  $\sqrt{3} \times \sqrt{3}$  structure, we measured the rocking curves along the  $[11\bar{2}]$  direction at 289 K, as shown by the open circles in Fig. 4(b). As described above, the vertical atomic positions remain unchanged above and below the phase-transition temperature. In considering the transformation from the  $2\sqrt{3} \times 2\sqrt{3}$  to  $\sqrt{3} \times \sqrt{3}$  periodicity, the lateral atomic positions should be changed upon the phase transition. Above the phase-transition temperature, it is considered that the K atoms are randomly distributed on the  $\text{Si(111)-}\sqrt{3} \times \sqrt{3}$ -B surface. Thus we calculated the RHEPD rocking curves assuming that the K atoms are randomly situated at the intermediate positions between the  $H_3$  and  $T'_4$  sites in the  $2\sqrt{3} \times 2\sqrt{3}$  unit cell. As shown by the solid lines in Fig. 4(b), the measured curve for each spot can be reproduced by the calculated curve using the randomly distributed model. Therefore the K atoms are disordered due to the phase transition.

From photoemission spectroscopy data, the low-temperature phase is considered to be the bipolaron phase.<sup>7,8</sup> In this phase, it is suggested that three of four Si adatoms are shifted to a higher position in the unit cell. Considering the charge transfer of  $1.0e^-$  per K atom determined in this study, it is likely that the atomic orbitals for the Si adatoms are changed from  $sp^2$  like to  $sp^3$  like. Therefore three of four Si atoms are expected to shift toward the vacuum region, in agreement with a previous photoemission study.<sup>8</sup> The K atoms are situated at the intermediate positions between the  $H_3$  and  $T'_4$  sites, giving rise to a higher adsorbed position. Hence the K atoms that are shifted to higher positions are loosely bound to the Si adatoms. Consequently, the  $\text{K/Si(111)-}2\sqrt{3} \times 2\sqrt{3}$ -B surface at low temperature is responsible for the bipolaronic phase and the  $\text{K/Si(111)-}\sqrt{3} \times \sqrt{3}$ -B surface at high temperature is in the disordered state.

#### IV. SUMMARY

In summary, we investigated the atomic structures and charge transfers of the  $\text{K/Si(111)-}2\sqrt{3} \times 2\sqrt{3}$ -B and  $\sqrt{3} \times \sqrt{3}$ -B surfaces using reflection high-energy positron diffraction. We found that the K atoms form a trimer structure on the  $\text{K/Si(111)-}2\sqrt{3} \times 2\sqrt{3}$ -B surface with charge transfer of  $1.0e^-$  taking place from the K to the Si atom. The Si adatoms are significantly shifted upward. When the temperature increases to above 270 K, the surface undergoes a phase transition from the  $2\sqrt{3} \times 2\sqrt{3}$  to the  $\sqrt{3} \times \sqrt{3}$  structure. The K atoms are randomly distributed on the  $\text{Si(111)-}\sqrt{3} \times \sqrt{3}$ -B surface at room temperature. Therefore this surface phase transition may be classified as an order-disorder phase transition with charge transfer.

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\*fukaya.yuki99@jaea.go.jp

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