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Surface structure of In/Si(1 1 1) studied by reflection high-energy positron diffraction

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Abstract

We have investigated a quasi-one-dimensional structure of In/Si(1 1 1) surface using reflection high-energy positron diffraction (RHEPD), which is sensitive to the topmost surface structure under the total reflection condition. From the rocking curves, we found that In atoms are located at two different vertical positions, i.e., 0.99 Å and 0.55 Å from the Si zigzag chain in both 4×1 (210 K) and 8×2 (60 K) phases.

Keywords: Surface structure; Reflection high-energy positron diffraction; Total reflection; Silicon; Indium

1. Introduction

Adsorption of In on Si(1 1 1) surface gives rise to various phases such as $\sqrt{3}\times\sqrt{3}R30°$, $\sqrt{31}\times\sqrt{31}R9°$, 4×1 and $\sqrt{7}\times\sqrt{3}$ depending on the coverage and the temperature. When the coverage is 1 monolayer (ML), a quasi-one-dimensional (1D) structure is formed [1,2]. This structure has 4×1 and 8×2 periodicities above and below 130 K [3–5]. The structure of the In/Si(1 1 1)-4×1 surface has been determined by surface x-ray diffraction (SXRD) [6] and μ-probe Auger electron diffraction (AED) [7]. As shown in Fig. 1, the one-dimensional In arrays along the $[1\,1\,\bar{2}]$ direction are separated by approximately 13.3 Å. Between the In arrays are zigzag Si chains. Each In array is composed of two zigzag chains. In atoms are located at the T_4 and on-top sites in one of the two zigzag chains. In atoms are located at the H_3 and on-top sites in the other zigzag chains. The vertical height of the two In atoms at the T_4 and H_3 sites was reported to be nearly the same [6,7]. The vertical heights of the two on-top sites may be slightly different [6]. The In atoms at the T_4 and H_3 sites are located relatively upper than those at the on-top sites. The other studies such as scanning tunneling microscopy (STM) [2], angle-resolved photoelectron spectroscopy (ARPES) [8], inverse photoelectron spectroscopy (IPES) [9], reflectance anisotropy spectroscopy (RAS) [10], XRD [11], low-energy electron diffraction (LEED) [12], and ab-initio calculations [13–17] confirmed this zigzag chain model.

The 4×1 and 8×2 phases show metallic and insulating features, respectively [3–5,8,18–20]. Thus, this phase transition is considered to be metal-insulator transition [4,20]. The structure of the 8×2 has not yet been determined although the 4×2 structure [21], which should be building blocks of 8×2 structure, was investigated [11]. Therefore, the phase transition mechanism between 4×1 and 8×2 structures is not fully clarified.

The advantage of reflection high-energy positron diffraction (RHEPD) [22,23] is the occurrence of total reflection. The RHEPD intensity is sensitive to the topmost surface structure under the total reflection condition. In this paper, we have investigated the atomic geometries of the In/Si(1 1 1)-4×1 and 8×2 surfaces.

2. Experiment

The sample was cut from a mirror-polished, 1–10 Ωcm, n-type Si(1 1 1) wafer. A clean Si(1 1 1)-7×7 surface was

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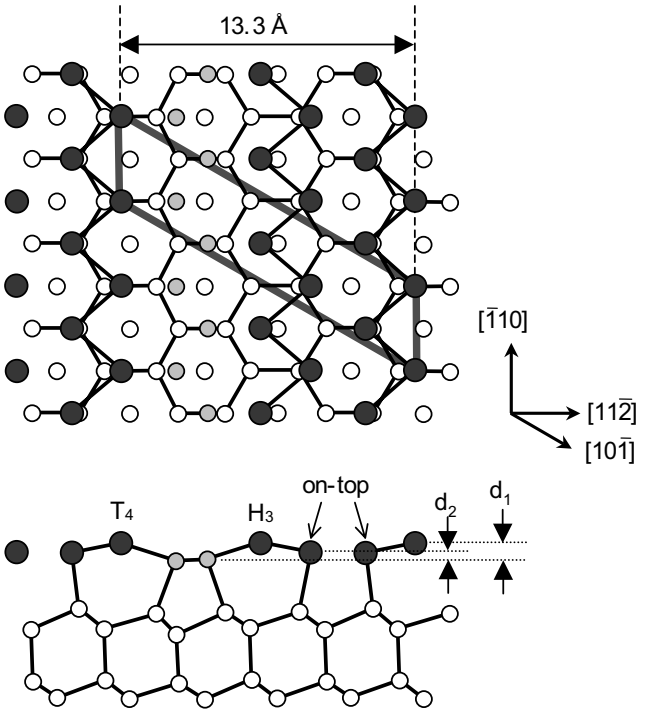

Fig. 1. Top and side view for In/Si(1 1 1)-4 × 1 surface. The large black circle is the topmost In atoms. Filled and open circles indicate first layer Si atoms and deeper layer Si atoms, respectively. d_1 and d_2 denote the heights of upper and lower In atoms from the first Si zigzag-chain layer, respectively. Parallelogram (15.4 Å × 3.8 Å) indicates a unit cell of 4 × 1 structure.

obtained by heating at 1470 K several times in an ultra-high vacuum (UHV) chamber at a base pressure of less than 5×10^{-8} Pa. The In/Si(1 1 1)-4 × 1 surface was formed by depositing 1 ML of In atoms on the Si(1 1 1)-7 × 7 surface at 670 K. After the deposition, the surface was annealed at 670 K for 1 min so as to obtain sharp 4 × 1 pattern in reflection high-energy electron diffraction (RHEED).

RHEPD experiments were carried out in a UHV chamber equipped with a ^{22}Na positron source and a magnetic lens system [24]. The positron energy was set at 10 keV. Rocking curves were obtained by changing the glancing angle of the incident beam from 0.3° to 6.0° with an interval of 0.1°. The azimuthal angle is 7.5°-off oriented from the [1 1 $\bar{2}$] direction. This is called the one-beam condition [25]. In the one-beam condition, the influence of simultaneous reflection parallel to the surface is sufficiently suppressed. Hence, the rocking curve depends only on atomic positions normal to the surface.

3. Results and discussion

Fig. 2 displays the rocking curves of specular spots measured from the In/Si(1 1 1)-4 × 1 (210 K) and 8 × 2 (60 K) surfaces. The critical angle for the total reflection is calculated to be 2.0° taking into account the inner potential (12 V) of Si crystal [25]. Up to the glancing angle of 3.5°, the intense peaks composed of the total reflection, the

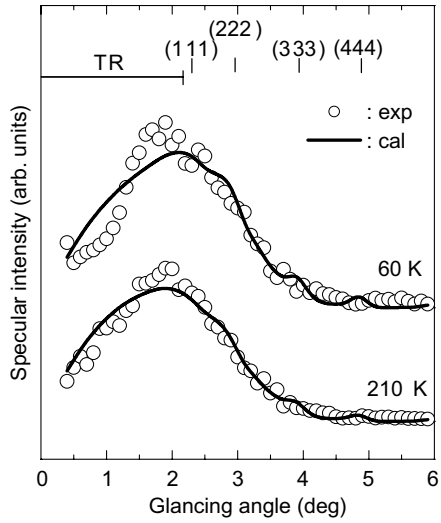

Fig. 2. RHEPD rocking curves from the In/Si(1 1 1) surface under one-beam condition at 60 K and 210 K. The open circle and the solid line show the measured and calculated rocking curves, respectively. The rocking curve was calculated based on the dynamical diffraction theory using the optimized geometries of the In atoms. TR stands for the total reflection region.

(1 1 1) and the (2 2 2) Bragg reflections are observed. The (3 3 3) and the (4 4 4) Bragg reflections are small. Although a slight drop of the intensity is seen below 1.2° in the case of 60 K, the overall shapes of the rocking curves at 60 K and 210 K are very similar to each other.

To determine the vertical positions of In atoms for the 4 × 1 and 8 × 2 phases, the rocking curves were analyzed using the dynamical diffraction theory [26]. The structure model determined by SXRD [6] was used in the simulations. The Debye-temperature of Si atoms was set to be 610 K [27]. The Debye-temperature of In atoms was assumed to be 108 K [12]. The absorption potentials for electronic excitations at In and Si layers were chosen to be 0 V and 1.70 V, respectively [28,29]. The vertical position of the Si zigzag chain was assumed to be 2.34 Å from the top Si atoms of unreconstructed substrate. The distances from the upper (d_1) and lower (d_2) In atoms to the Si zigzag chain (see Fig. 1) were changed so as to minimize the difference between the measured and calculated curves. The goodness of the fitting was judged using the reliability factor defined in Ref. [27].

The solid lines show the calculated rocking curves using the optimized geometries at each temperature. The measured rocking curves are in good agreement with the calculated curves at both temperatures. The vertical distances from the In atoms to the Si zigzag chain are listed in Table 1. The vertical distances from the upper (d_1) and lower (d_2) In atoms to the Si zigzag chain at 210 K were determined to be 0.98 ± 0.09 Å and 0.54 ± 0.09 Å, respectively. Comparing these values with those determined in other studies in Table 1, the values obtained in this study are slightly higher than those by SXRD [6] and ab-initio calculations [15,16]. We found that our values are close to those obtained by LEED [12] and ab-initio calculation [13].

Table 1
Vertical distances from the upper (d_1) and lower (d_2) In atoms to the first Si zigzag-chain layer for the In/Si(1 1 1)-8 × 2 (60 K) and 4 × 1 (210 K) surfaces

Parameter	Present (60 K)	Present (210 K)	SXRD [6]	LEED [12]	Ab-initio [13]	Ab-initio [15]	Ab-initio [16]
d_1 (Å)	0.99 ± 0.09	0.98 ± 0.09	0.76	0.86	0.87	0.77	0.76
d_2 (Å)	0.55 ± 0.10	0.54 ± 0.09	0.34	0.49	0.45	0.33	0.39

Also, the vertical distances from the upper and lower In atoms to the Si zigzag chain at 60 K were determined to be 0.99 ± 0.09 Å and 0.55 ± 0.10 Å, respectively. The values are almost the same as those at 210 K. We found that the heights of the upper and lower In atoms do not change with temperature. This is consistent with the result of RAS [10], LEED [12], and ab-initio calculations [16]. Therefore, the heights of the In atoms for the 4×1 and 8×2 phases are almost the same. It is considered that the difference of the atomic positions between the 4×1 and 8×2 phases appears in the direction parallel to the surface. Detailed understanding of the displacements of the atomic positions is important for revealing the mechanism of the phase transition from the 4×1 to 8×2 phase.

4. Summary

In summary, we have investigated the 1D structure of In/Si(1 1 1) surface using RHEPD. We measured the rocking curves from the In/Si(1 1 1)-4 × 1 (210 K) and 8 × 2 (60 K) surfaces. The rocking curve for the specular spots did not change with the temperature (60 K and 210 K). We found that the vertical distances from the upper and lower In atoms to the Si zigzag chain are conserved during the phase transition.

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