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Reflection high-energy positron diffraction study of a Si(0 0 1) surface

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Abstract

We have studied the positron diffraction from the Si(0 0 1) 2 × 1 surfaces. In the diffraction patterns the fractional order spots are brightly visible. The vertical positions of the dimer are determined from the numerical analysis of the rocking curves based on the dynamical diffraction theory at room temperature and 130 K. The heights of the two atoms of the dimer are both 1.3 ± 0.2 Å at room temperature and 1.3 ± 0.2 Å and 1.1 ± 0.2 Å at 130 K from the layer below the dimers.

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Keywords: Reflection high-energy positron diffraction; Total reflection; Si(0 0 1); Rocking curve; Dynamical calculation; Diffraction pattern

1. Introduction

The Si(0 0 1) clean surface shows a phase transition between 2 × 1 and $c(4 \times 2)$ at around 200 K [1,2]. This is generally described by an order–disorder transition. At low temperature, the two atoms in the dimer freeze in the asymmetric dimer configurations according to many experimental and theoretical reports [3–7]. A flip-flop motion between two equivalent asymmetric dimer configurations is thermally activated above 200 K [8,9]. To understand a series of the phase transition in the Si(0 0 1) surfaces, it is important to determine the atomic positions of the surface. At room temperature many studies, such as reflection high-energy electron diffraction (RHEED) [10,11], low-energy electron diffraction (LEED) [12,13], medium energy ion scattering (Ion beam) [14] and so on, have revealed the atomic structures of the Si(0 0 1) 2 × 1 surfaces. There are, however, a few studies in order to investigate the atomic positions of the $c(4 \times 2)$ structure below 200 K [15].

Reflection high-energy positron diffraction (RHEPD) is a new and powerful technique to investigate topmost atomic structures and thermal vibrations [16–23]. Positrons are totally reflected at the topmost surfaces, when the glancing angle is

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below a critical angle, because of the positive crystal potential for positrons [16]. The shape of rocking curve in the total reflection region is quite sensitive to the changes of the atomic structures on the surfaces [17–22].

In this study, we have observed the world's first RHEPD patterns from the Si(0 0 1) clean surface at room temperature and 130 K. The vertical positions of dimer atoms are determined by the analysis of the RHEPD rocking curves.

2. Experimental

The specimens (0.5mm × 5mm × 10 mm) used in this study were cut from a p-type Si(0 0 1) wafer (3000 Ω cm). These were cleaned in a pure ethanol and subsequently were transferred into an UHV chamber evacuated to a base pressure of 5×10^{-8} Pa. After degassing processes at about 700 K for several hours, the sample flashing was carried out at 1500 K for 10 s a few times by a direct current flow. After the final flashing, the samples were cooled at 2 or 3 K/s to about 500 K. The formation of the Si(0 0 1) 2 × 1 surface was confirmed by RHEED.

RHEPD experiments were performed using a positron beam with an energy of 10 keV. The details of the apparatus are described elsewhere [23]. The rocking curves were measured at the glancing angle from 0.1 to 7.5° with a step of 0.1° at room temperature and 130 K. The azimuthal angle was fixed at 24° from the [1 1 0] direction. This is so called the one-beam condition where approximately only the specular beam is observed [10,24]. Measuring time for a rocking curve was three hours and a half.

3. Results and discussion

Fig. 1 shows the experimental RHEPD pattern at the [1 1 0] direction and at the glancing angle of 1.3° at room temperature. Taking the crystal potential as 12 keV [24], the critical angle for the total reflection is 2.0° according to the Snell's equation. Two strong spots are assigned to the $1/2, 0$ and $\overline{1/2}, 0$ reflections. This is consistent with the RHEED observation which shows the appearance of the 2 × 1 periodicity. Although the $c(4 \times 2)$ structure was observed at low temperatures using scanning tunneling microscopy, RHEPD patterns did not show such periodicity. This is probably due to the limitation coming from the beam coherence length.

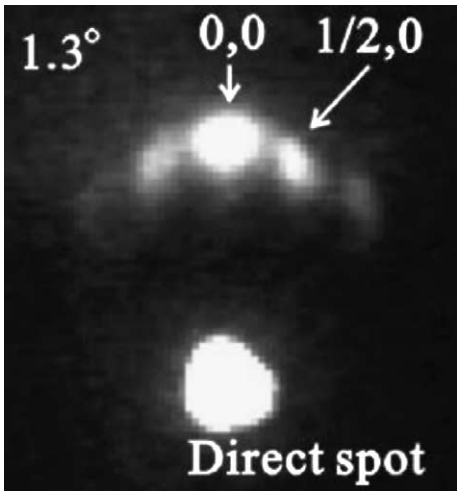

Fig. 1. The experimental RHEPD pattern at room temperature from the Si(0 0 1) 2 × 1 clean surface at the [1 1 0] direction and at the glancing angle of 1.3°.

Fig. 2 shows the rocking curves of the specular spot under the one-beam condition at room temperature and at 130 K. Both rocking curves exhibit two large

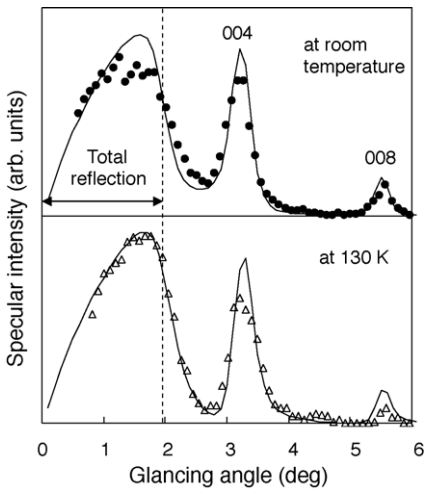

Fig. 2. The rocking curves of the specular spot at 24° away from the [1 1 0] direction under the one-beam condition at room temperature and at 130 K. Solid lines are the best curves in the calculations based on the dynamical diffraction theory.

Table 1
The vertical distances $d_a = d1 - d3$ and $d_b = d2 - d3$ about the present and the other studies

	Present		Ion beam	RHEED	LEED		Theory[e]
	RT	130 K	RT[a]	RT[b]	RT[c]	80 K[d]	
d_a(Å)	1.3 ± 0.2	1.3 ± 0.2	1.38	1.38	1.13,1.45	1.44	1.18,1.39
d_b(Å)	1.3 ± 0.2	1.1 ± 0.2	0.91	0.81	0.69,1.05	0.70	0.94,0.69

[a] Ref. [14] (at room temperature).
[b] Ref. [10] (at room temperature).
[c] Refs. [12,13] (at room temperature).
[d] Ref. [15] (at 80 K).
[e] Refs. [6,7].

peaks at 1.5° and 3.3°, and one small peak at 5.6°. The first peak corresponds to the total reflection. The second and third peaks are assigned to the 004 and 008 Bragg reflections, respectively. One clear difference of the rocking curves between at room temperature and at 130 K is noticed for the peak structure of the total reflection peak. That is, the intensity at 130 K is greater than that at room temperature. The other difference is the shape of the dip at 2.7°. The intensity at 130 K is weaker than that at room temperature.

The above rocking curves were analyzed using the numerical calculations based on the dynamical diffraction theory. In order to compare the calculations with the experiments, the reliability factor R is expressed as $R = \sqrt{\sum_\theta (I_\theta^{\exp} - I_\theta^{\mathrm{cal}})^2}$ $(\sum I_\theta^{\exp} = \sum I_\theta^{\mathrm{cal}} = 100\%)$, where $I_\theta^{\exp}$ is the experimental intensity and I_θ^{cal} calculated one at the glancing angle θ. In the calculations, since the shapes of the rocking curves are sensitive to $d1$, $d2$ and $d3$ as shown in Fig. 3, we optimized $d1$, $d2$ and $d3$ with the other atomic positions fixed. Solid lines shown in Fig. 2 are the best rocking curves to reproduce the experiments. We obtained $d1$, $d2 = 2.7$ Å and $d3 = 1.4$ Å with the minimum value of $R = 3.4\%$ at room temperature, and $d1 = 2.7$ Å, $d2 = 2.5$ Å and $d3 = 1.4$ Å with the minimum value of $R = 2.8\%$ at 130 K within the error range ±0.2 Å. The atomic positions of the dimer are approximately the same value at both temperatures within the error range. Table 1 lists the vertical distances of the individual dimer atoms from the second layer, $d_a = d1 - d3$ and $d_b = d2 - d3$, determined in the present and the other studies. The present values of d_a are in agreement with the other results at room and low temperatures within the error range. The present values of d_b are larger than the other results at both temperatures. Although the reason for these discrepancies is not clear at present, we consider the possibility of the influence of contamination on the surface. Since the Si(0 0 1) clean surfaces are sensitive to contamination, a little contamination may be absorbed to the surfaces for a few hours of the measuring time. To clarify this possibility the further study is needed.

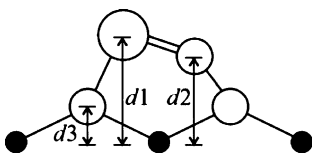

Fig. 3. Definition of the interlayer distances for the Si(0 0 1) 2 × 1 structure.

4. Summary

We investigated the clean Si(0 0 1) 2 × 1 surface using RHEPD at room temperature and at 130 K. The diffraction spots coming from the 2 × 1 structure are clearly observed in the pattern. By the analysis of the rocking curves, it is found that the atomic vertical positions of the dimer are approximately the same value at both temperatures within the error range.

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