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Reflection high-energy positron diffraction pattern from a Si(1 1 1)-(7 × 7) surface

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Abstract

We have investigated the feature of reflection high-energy positron diffraction (RHEPD) pattern from a Si(1 1 1)-(7 × 7) surface. The RHEPD pattern observed in the total reflection condition is quite different from the conventional reflection high-energy electron diffraction (RHEED) pattern. This fact is attributed to the different penetration depths of positrons and electrons. We show that the intensity distribution of RHEPD pattern is reproduced considering the dimer-adatom-stacking fault (DAS) model with optimized atomic positions and scattering potentials of adatoms and rest atoms.

Keywords: Reflection high-energy electron diffraction (RHEED); Surface structure, morphology, roughness, and topography; Silicon; Low index single crystal surfaces

1. Introduction

The structure of Si(1 1 1)-(7 × 7) reconstructed surface has been intensively studied [1–9] since its discovery by low-energy electron diffraction (LEED) [1]. Binnig et al. revealed the existence of twelve adatoms using scanning tunneling microscopy (STM) [2]. Subsequently Takayanagi et al. proposed the dimer-adatom-stacking fault (DAS) model based on the analysis of transmission electron diffraction pattern [3]. This model is supported by the later studies using reflection high-energy electron diffraction (RHEED) [4], LEED [5], X-ray diffraction (XRD) [6,7], and theoretical calculations [8,9]. Although the structure of Si(1 1 1)-7 × 7 surface is nearly fully solved, we attempt to reexamine it using newly developed reflection high-energy positron diffraction (RHEPD) in the present work.

An exceptional feature of RHEPD is the total reflection which never occurs in electron diffraction. In the total reflection condition [10], positrons hardly penetrate into the bulk [11]. Recently, using RHEPD rocking curve, the adatom height of Si(1 1 1)-(7 × 7) reconstructed surface was determined to be 1.52 Å [12]. This value is greater than that determined by RHEED [4] and LEED [5], while in good agreement with that obtained by the XRD [6,7]. It is demonstrated from the temperature dependent RHEPD intensities in the total reflection condition that the thermal vibration amplitude of adatoms is greater than that determined from the RHEED study [13,14]. We also investigated the RHEPD patterns of Si(1 1 1)-(7 × 7) surface with kinematical diffraction theory [15]. It is found that the kinematical calculation reproduces the observations qualitatively, but not quantitatively. Therefore, the dynamical calculation is necessary to estimate the diffraction intensities precisely.

In the present research, we show how the RHEPD pattern of Si(1 1 1)-(7 × 7) is different from the RHEED pattern and how it is reproduced by dynamical diffraction theory with an optimized atomic coordinate and scattering potentials associated with the surface layer.

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2. Experimental

Specimen ($10 \times 5 \times 0.5\ mm^3$) was cut from an n-type Si(1 1 1) wafer with a resistivity of 10 Ω cm. The specimen was cleaned in pure ethanol and subsequently transferred to an UHV chamber, evacuated to a base pressure of 5×10^{-8} Pa. Following the degassing processes conducted at approximately 700 K for several hours, the specimen was heated at 1500 K for 10 s a few times by a direct current flow. The formation of a Si(1 1 1)-(7 × 7) periodicity was confirmed by RHEED. Well-focused positron beam with energy of 10 keV was irradiated onto the specimen surface at the glazing incidence with an angle of 1.95° and from the $[1\,1\,\bar{2}]$ direction, and reflected positrons were observed using a micro-channel plate assembly (Hamamatsu F2226–24P) and a charge-coupled device (CCD) camera. The glancing angle satisfies the total reflection condition (<1.99°).[1] The CCD flame images were digitally accumulated for 6 h. The details of the apparatus are described elsewhere [16].

3. Results and discussion

Fig. 1(a) shows the observed RHEPD pattern. The open circles denote the expected positions of the integer-order spots in the first Laue zone. The inset at the lower left corner shows the pattern in the area surrounded by the broken lines. The zeroth Laue zone in the pattern includes seven bright spots as denoted by (0,0), $(1/7,1/7)$, $(\overline{1/7},\overline{1/7})$, $(2/7,2/7)$, $(\overline{2/7},\overline{2/7})$, $(3/7,3/7)$ and $(\overline{3/7},\overline{3/7})$. The 1/7th Laue zone is also clearly observed in the pattern. The $(3/7,4/7)$ and $(\overline{4/7},\overline{3/7})$ spots have the strongest intensities in this zone. It should be noted that most of spots between the 2/7th and the first Laue zones are very weak. This feature is quite different from the case of RHEED pattern where clear spots appear even in the higher-order Laue zones as described later.

We now attempt to reproduce the RHEPD pattern through the computation based on the dynamical diffraction theory [17]. As shown in Fig. 2, we take 519 beams, which cover all the spots in the fluorescent screen and the same area of the negative Laue zones [18]. The Debye temperatures of adatoms and the bulk atoms are assumed to be 290 K and 600 K, respectively [13,14]. The shape of imaginary potential for the thermal diffuse scattering is approximated by Gaussian distribution function [17,19]. The Debye parameter B and the imaginary potential for thermal diffuse scattering v_0^{TDS} are 1.50 Å^2 and 0.71 V for the adatom, and 0.38 Å^2 and 0.37 V for the other atoms, respectively. The imaginary potentials for electronic excitations are assumed to be 0.25 V for adatoms [12] and 1.24 V

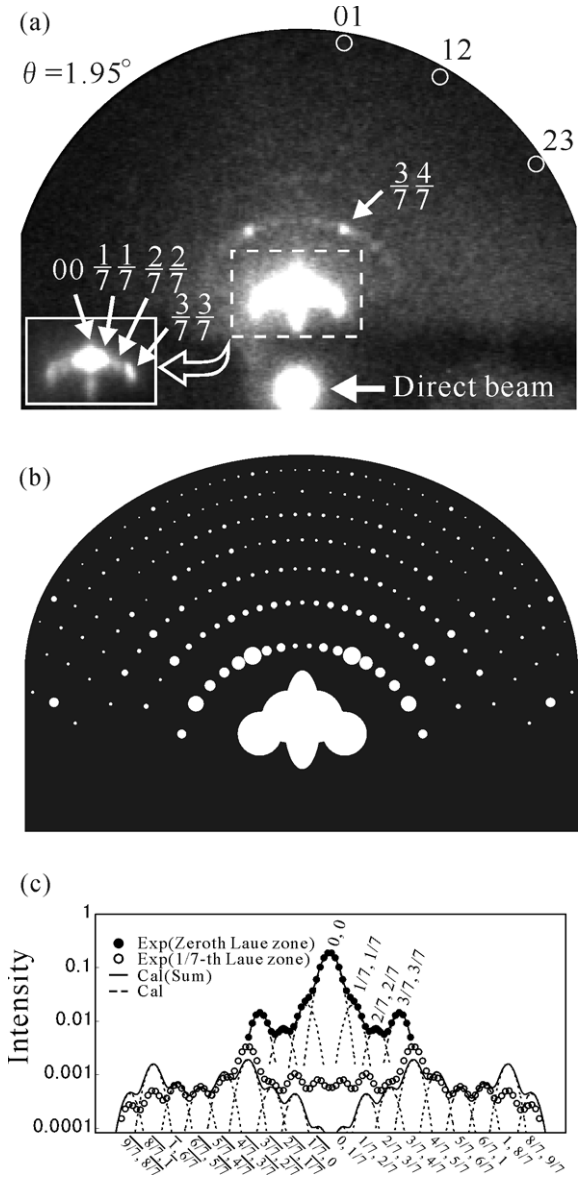

Fig. 1. RHEPD patterns obtained in (a) experiment and (b) calculation in the total reflection from a Si(1 1 1)-(7 × 7) at the $[1\,1\,\bar{2}]$ direction and at the glancing angle of 1.95°. (c) Intensity profiles along the zeroth Laue zone and the 1/7th Laue zone. Solid and open circles denote the experimental results along the zeroth and the 1/7th Laue zone, respectively. Broken and solid lines show the calculated profiles for individual spots and their summation, respectively. The calculated spots are convoluted by Gaussian distribution function with the FWHM of 0.3°. The peak intensity of the specular spot is normalized to unity.

for the others atoms [4,17]. As for the atomic positions as shown in Fig. 3, we optimized the adatom positions (d_1, s_1 and s_2). The others ($d_2 - d_6$) are the same as previous works [4,20] because the displacements from their values have only a minor role for calculated spot intensities. The optimized values are $d_1 = 1.53$ Å, $s_1 = 0.00$ Å and $s_2 = 0.03$ Å for the minimum value of least square between the calculated spot intensities and the experimental ones in the zeroth and the 1/7th Laue zones. The height of adatoms ($d_1 = 1.53$ Å) is in good agreement with 1.52 Å which

[1] The critical angle θ_c of the total reflection is given by $\theta_c = \arcsin(V_0/E)^{1/2}$, where V_0 is the crystal potential and E is the incident positron energy. In the present experiment, since the value of eV_0 is 12 eV for silicon and the value of E is 10 keV, the critical angle θ_c is estimated to be 1.99°.

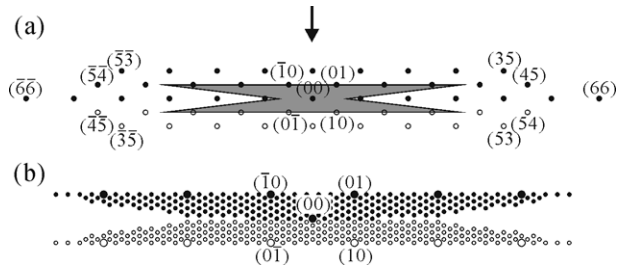

Fig. 2. A top view of the sets of reciprocal rods of Si(1 1 1)-(7 × 7) used for the dynamical calculations. (a) The reciprocal rods with the indices of the integer number. The gray area consists of the fractional order rods. (b) The reciprocal rods with the fractional indices. The solid and open circles denote the reciprocal rods in the positive (including zero) and negative Laue zones, respectively. The arrow indicates the direction of the incident beam.

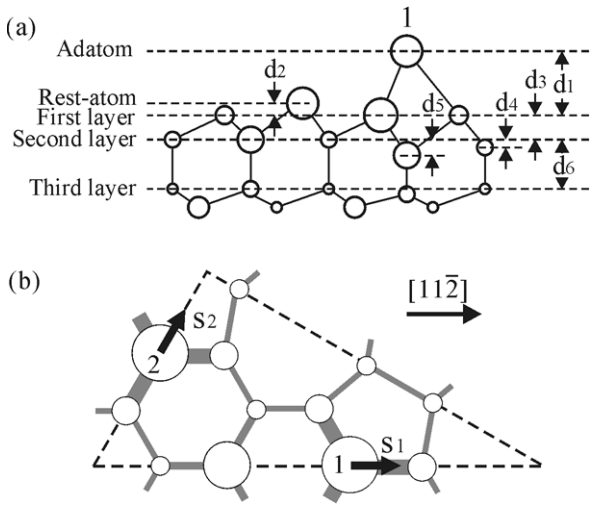

Fig. 3. A schematic illustrations of the atomic positions of the DAS model of (7 × 7) surface at (a) the [0 1 $\bar{1}$] side view and (b) the top view. The adatom numbered 1 adjoins the corner hole of a DAS structure and the adatom numbered 2 lies between the No. 1 adatom and the symmetric No. 1 adatom. The arrows and *s* show the directions and the distances of the displacement, respectively.

is determined by the previous analysis of RHEPD rocking curve [12]. The lateral displacements (s_1 and s_2) are almost the same value as the other results using RHEED [4], LEED [5] and XRD [6,7]. Our calculation result about the adatom positions is consistent with the previous results. In the calculations for the optimization, we found that, to obtain an RHEPD pattern comparable to the observation, the scattering (real parts) potentials for adatoms and rest-atoms should be varied from those by Doyle and Turner (DT) [21]. We obtained the optimized surface potential drawn in Fig. 4. The potential responsible for the adatom layer is by approximately 30% larger than the DT potential, while that for the rest atom layer is by approximately 20% smaller than the DT potential. Thus, adatoms act as relatively stronger scattering centers and rest atoms as weaker scattering centers as compared to free Si atoms.

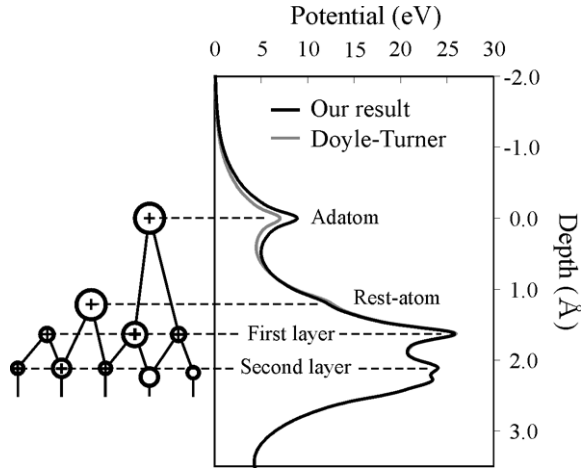

Fig. 4. Curves of projection potentials of Si(1 1 1)-(7 × 7) DAS surface as a function of the depth from the surface. The black solid line denotes the optimized curve to reproduce the experimental pattern. The gray solid line denotes the simple Doyle–Turner potential.

Considering the formula of the scattering potential of an atom,[2] this is probably due to the changes in their scattering potentials because of the charge-transfer from adatoms to rest-atoms as proposed by Avouris and Wolkow [22]. The calculated pattern is shown in Fig. 1(b). Here, the areas of the circles are proportional to the relative intensities of the diffraction spots. The shape of (0 0) spot is an artifact because the circle of the (0 0) spot with strong intensity is too large to draw in the figure. The intensity profiles for the zeroth and the 1/7th Laue zones are also drawn in Fig. 1(c) with experimental data. The calculation well reproduces the experiment. This assures the validity of above calculation.

As stated above, the intensities of fundamental spots in the first Laue zone are very weak in the RHEPD pattern. This is obviously different from the case of the RHEED patterns (see, for example, Ref. [20]). Such a clear difference is attributed to the different penetration depths of positrons and electrons. The penetration depth of positrons is extremely small in the total reflection region.[3] Therefore, the large thermal vibration of adatoms weakens the higher order spot intensities. If we use the same Debye

[2] The scattering potential of an atom $V(r)$ is given by, $V(r) = \frac{Ze}{r} - e\int \frac{\rho(r')}{|r-r'|}\mathrm{d}\tau'$, where Z is the atomic number, $\rho(r)$ is the charge density at r from the center of atom and $\mathrm{d}\tau'$ is the infinitesimal volume. Thus, total potential is enhanced (moderated) due to the decrease (increase) of the charge density. Therefore, the enhanced and moderated potentials for adatoms and rest-atoms shown above may correspond to the charge transfer from adatoms to rest-atoms.

[3] The calculated spot intensities hardly change for the displacement of the distance d_3 between the first and the second layer. This means that the incident positrons barely reach the atoms below the second layer. Therefore, we estimated the penetration depth of positrons at less than 2.1 Å ($=d_1 + d_3$). The value is in agreement with that (the penetration depth $l = 3$ Å) estimated by Snell's law ($l = 1/\sqrt{2\pi|k - V_0|}$) without the effects of adsorption, where k is the surface normal component of an incident wave in vacuum and V_0 is a mean inner potential.

temperature for adatoms as bulk atoms, the intensities of integer order sports in the first Laue zone increase to comparable level to RHEED. In the case of RHEED, the incident electrons are refracted at the surface layer and penetrate into the bulk layers. Therefore, the higher order spots appear more clearly as the effect of bulk.

4. Summary

We observed the RHEPD pattern from a Si(1 1 1)-(7×7) surface at the total reflection condition. The calculated RHEPD pattern using the dynamical diffraction theory is in good agreement with the experimental one. The spot intensities mainly depend on the position and thermal vibration of adatoms. It is indicated that the scattering potentials of adatoms and rest-atoms are different from those of free silicon atoms. Weak intensities of the higher-order diffraction spots are attributed to the large thermal vibration of adatoms.

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