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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

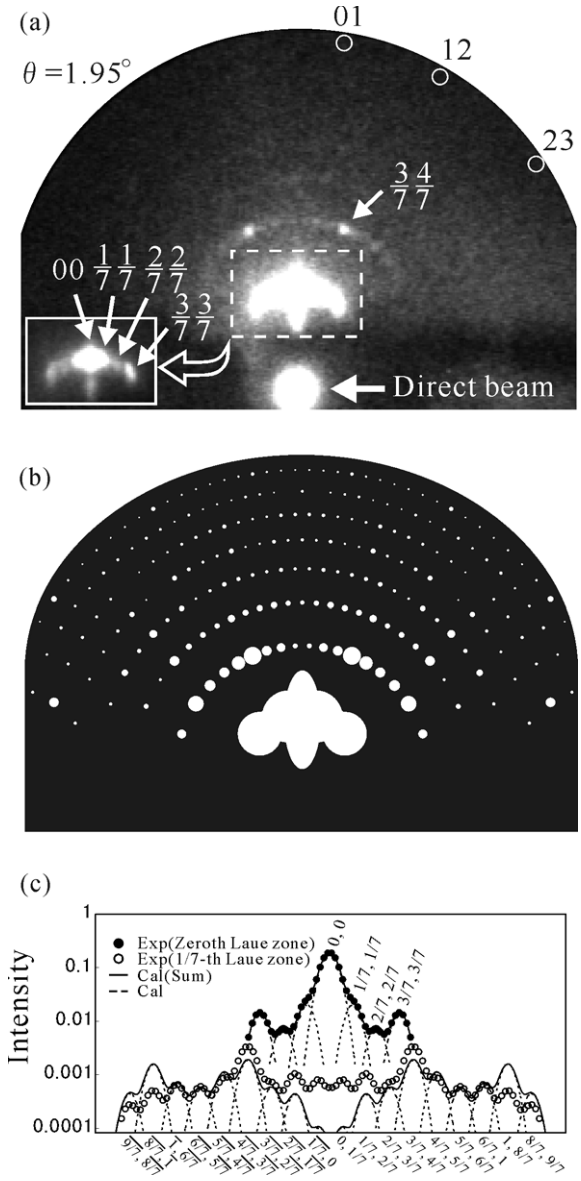

Fig. 1. RHEPD patterns obtained in (a) experiment and (b) calculation in the total reflection from a Si(1 1 1)-(7 × 7) at the $[1\,1\,\bar{2}]$ direction and at the glancing angle of 1.95°. (c) Intensity profiles along the zeroth Laue zone and the 1/7th Laue zone. Solid and open circles denote the experimental 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°.