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Reflection high-energy positron diffraction at solid surfaces by improved electrostatic positron beam

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Abstract

We report observation of reflection high-energy positron diffraction (RHEPD) at the Si(1 1 1) surface using an electrostatic positron beam. The improvement of the beam (i.e., reduction of beam energy spread) was critical to obtaining the higher-order diffraction spots. We could observe the first Laue zone, which was not seen in our previous work. This allows us to study the surface Debye temperature. The obtained rocking curve represents the enhancement of the fourth Bragg peak, as expected from diffraction theory, in addition to previously confirmed total reflection and the first Bragg peak. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Reflection high-energy positron diffraction; Surface; Dipole barrier; Laue zone

1. Introduction

In reflection high-energy positron diffraction (RHEPD) experiments, back-reflection of high-energy (>10 keV) positrons at solid surfaces is observed at small glancing angle (<5°) [1]. Positrons are diffracted at the surface and the observed pattern represents reciprocal lattice rods related to surface atomic arrangement. The method itself is just the same as reflection high-energy electron diffraction (RHEED). Because of positive crystal potential for positrons, positrons are totally reflected at the topmost surface below a critical angle $\theta_C = \arcsin(eV_0/E)^{1/2}$, where eV_0 is the crystal potential and E the incident positron energy [2]. Total reflection is never observed in RHEED experiments due to negative crystal potential for electrons. A positive crystal potential also leads to an appearance of the first Bragg peak even if it is not observed in RHEED [2]. From an analysis of the positron reflectivity in the total reflection region, one can determine the bond length of adsorbed atoms in the topmost surface without disturbance from the bulk layer. Moreover, surface lattice vibration and surface roughness can be determined. These are always problematic in the case of electron diffractions because electrons penetrate deep into the crystal. It is also proposed that the metal surface dipole barrier can be directly measured by RHEPD by taking advantage of the negligible exchange–correlation interaction [3]. The metal surface barrier is an important physical quantity related to the work function.

In 1998, we performed a RHEPD experiment in which diffraction patterns from a Si(1 1 1) surface were observed and rocking curves were determined [4].

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The total reflection intensity measurement of RHEPD has been extensively applied in surface studies [1]. The lowest (i.e., zeroth) order Laue zone can be readily observed as long as the surface is well finished. However, higher-order Laue zones have not yet been observed. This is a disadvantage when studying surface melting problems since the first Laue zone is associated with information related to the surface Debye temperature. The reason why the first Laue zone is missing in past works is most likely due to the spread of the incident positron energy, i.e., poor coherence length. To reduce the energy spread of the beam, we modified the earlier RHEPD apparatus by adding a hemispherical electrostatic analyzer and two Einzel lenses [5]. As a result, beam energy spread was reduced to below 1%. Using a long-length collimator, the angular divergence was reduced to less than 0.1°. In this article, we report how modification of the RHEPD apparatus has improved the results obtained.

2. Experiment

Samples used in this study were floating-zone grown Si(1 1 1) finished with a 40% NH_4F solution. It was confirmed that the surface dangling bonds are terminated with atomic hydrogen. The samples were placed in a vacuum chamber with a base pressure of 9×10^{-8} Pa. A well-collimated monochromatic positron beam of energy 20 keV was generated using an electrostatic method with ^{22}NaCl source (370 MBq) and a well-annealed tungsten moderator (6 μm) described elsewhere [5]. The sample was irradiated by the positron beam and back-reflected beams were detected by a microchannel plate assembly (Hamamatsu, F2226-24P) as shown in Fig. 1. Rocking curves (positron reflectivity versus glancing angle plot) were determined.

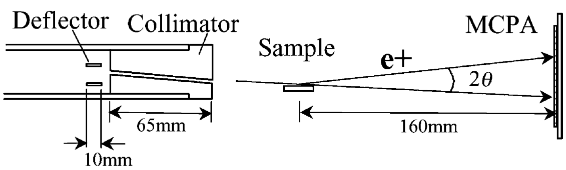

Fig. 1. Schematic drawing of the RHEPD experimental setup.

3. Results and discussion

As described above, only the zeroth Laue zone was observed before an improvement in the beam quality. This is speculated to be due to a poor energy resolution and the resultant reduction in the coherence length. Since in the present work the beam energy spread is reduced below 1% one may expect the appearance of fine structure in the diffraction pattern. Fig. 2(a) shows the RHEPD patterns for Si(1 1 1) surface finished with 40% NH_4F solution for $[1\,1\,\bar{2}]$ incidence at $\theta = 4.0°$. This figure was taken after integration for approximately 4 h. The lowest spot is the direct beam, which is not reflected at the surface. Here, one can see that in addition to the strong zeroth Laue zone ($(\bar{1}\,\bar{1})$, (0 0) and (1 1)), the first Laue zone appears in the high angle region. The indexes of the spots are $(\bar{3}\,\bar{4})$, $(\bar{2}\,\bar{3})$, $(\bar{1}\,\bar{2})$, $(0\,\bar{1})$, (1 0), (2 1), (3 2) and (4 3), as written in the figure. That is, these spots correspond to the reciprocal lattice rods shown in Fig. 2(b). The first Laue zone could not be observed in the past work [6]. The spot shape seems to be somewhat slender in the radial direction. This indicates residual energy spread. Nevertheless, the above results indicate that positron diffraction should give rise to essentially the same information as electron diffraction.

The first Laue zone could easily be observed at $\theta = 2$–$4°$ in our experiments. Although below this angle its intensity drastically decreased, a track of the first Laue zone could be still seen.

Fig. 3 shows the continuous photography of diffraction pattern in the zeroth Laue zone from 0.5° to 4°. Here, one can readily see that the diffraction intensity changes with screen position, i.e., glancing angle. Low background allows unambiguous determination of rocking curves for different diffraction spots. Fig. 4 shows the rocking curves for specular (0 0) and (1 1) spots. The peak at $\theta = 1.6°$ is assigned to the first Bragg peak which is unique for RHEPD experiments. The peak at around $\theta = 2.1°$ is due to the second Bragg peak which appears due to dynamical effects. The third to fifth Bragg peaks are successively observed at $\theta = 2.7°$, 3.5° and 4.2°, respectively. At $\theta < 1.4°$, total reflection of positrons occurs. At $\theta = 1.2°$, a dip appears which was previously interpreted as an interference effect due to surface roughness. The above features are qualitatively the same as those obtained in previous work [7]. The intensity of the fourth Bragg peak is higher than

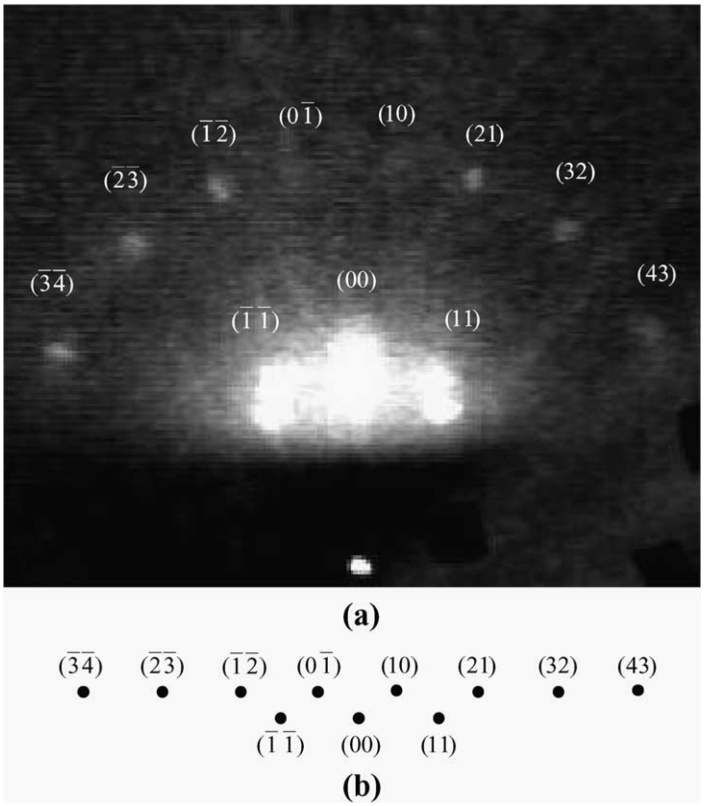

Fig. 2. (a) RHEPD pattern from Si(1 1 1) surface treated with NH_4F solution for the $[1\,1\,\bar{2}]$ incidence at glancing angle of 4.0°. (b) Reciprocal lattice of bulk truncated Si(1 1 1) surface which corresponds to diffraction indices shown in Fig. 1(a).

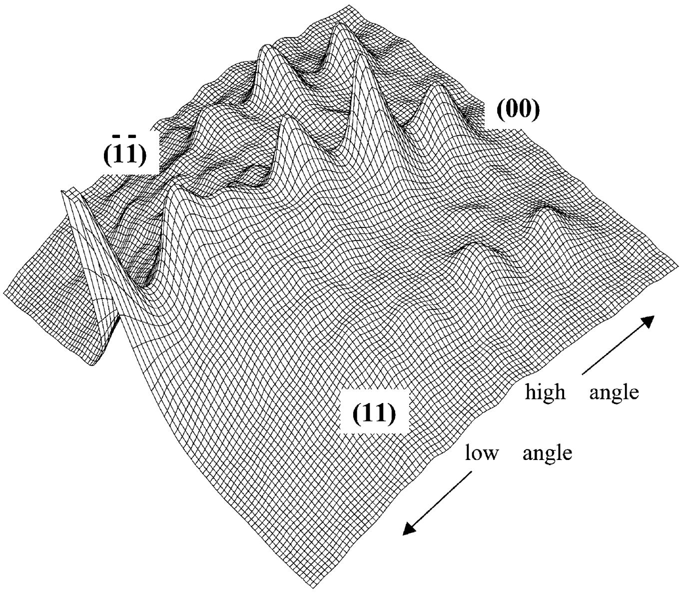

Fig. 3. A continuous photography of the zeroth Laue zone from Si(1 1 1) surface treated with NH_4F solution for the $[1\,1\,\bar{2}]$ incidence at $\theta = 0.5{-}5°$.

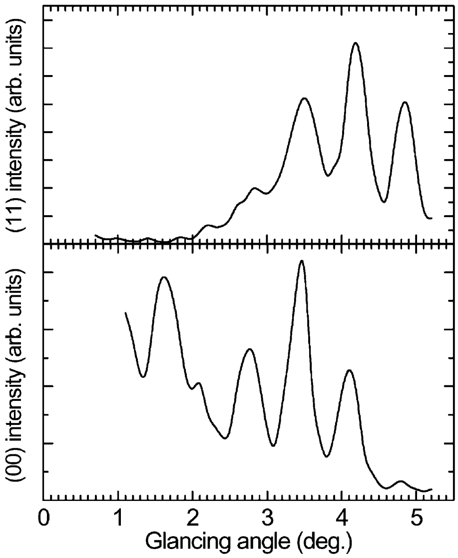

Fig. 4. Rocking curves of the (0 0) and (1 1) spot from Si(1 1 1) surface treated with NH_4F solution for the $[1\,1\,\bar{2}]$ incidence.

those of the third and fifth Bragg peaks. The enhancement of the fourth Bragg peak is anticipated within the kinematical theory where diffraction intensity has a maximum for $h + k + l = 4m$ (m is an integer). This effect was not confirmed in previous work.

Thus, the appearance of the first Laue zone suggests that the improvement of beam quality is crucial for examining fine structure in positron diffraction patterns. From dynamical diffraction theory, the first Laue zone is necessary to analyze surface Debye parameters. Furthermore, it is important to observe the first Laue zone in the total reflection region. Otherwise, the obtained Debye parameter is an admixture of surface and bulk components. The observation of the first Laue zone at low glancing angles, therefore, gives us future opportunities to measure the surface Debye parameter.

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