

## Total reflection positron diffraction from topmost layer of crystal surface

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### 1 Introduction

Reflection high-energy positron diffraction (RHEPD) is a surface-sensitive tool owing to the total reflection of positrons [1]. In 1998, we developed the RHEPD apparatus based on a <sup>22</sup>Na positron source [2]. Using the RI-based apparatus, we investigated the surface structures and the surface phase transitions of important systems. Recently, we developed a new RHEPD apparatus using intense and high-brightness positron beam generated from an electron linear accelerator (linac) to overcome a low flux of the RI-based beam. Using this apparatus, we succeeded in observing clear diffraction patterns of positrons from a crystal surface under the total reflection condition.

### 2 Experiment

Experiments were performed at the Slow Positron Facility, Institute of Materials Structure Science, KEK [3]. The intense positron beam was generated from the dedicated linac. A remoderator composed of 100-nm-thick W foil was utilized to enhance the brightness of the positron beam. The beam flux of the remoderated positron beam was estimated to be  $\sim 10^5$  e<sup>+</sup>/sec. The energy spread at the positron energy of 10 keV was 8 eV. The beam radius was less than 1.0 mm (FWHM).

A Si(111) surface was used as a sample, which was cut from a mirror-polished *n*-type wafer with a resistance of 1-10 Ωcm. They were flushed at 1200 °C in a ultra-high vacuum chamber to produce a 7×7 reconstructed structure.

### 3 Results and Discussion

Figure 1 shows the RHEPD pattern from the Si(111)-7×7 surface under the total reflection condition. The critical angle of the total reflection for positrons is evaluated via Snell's law. When the incident positron energy and the mean inner potential of Si are 10 keV and 12 eV, respectively, the critical angle corresponds to be 2.0°. As a result, we succeeded in observing clearer RHEPD patterns from the Si(111)-7×7 surface. The fractional-order spots in the high-order Laue zones are clearly observable, which have been never seen in the pattern using the <sup>22</sup>Na source. The measurements of RHEPD rocking curves were also successful. The intensity was 64 times as large as the <sup>22</sup>Na source method.

We calculated the diffraction pattern of positrons under the total reflection condition based on the dynamical diffraction theory. The calculated pattern under the total reflection condition does not almost depend on the atomic positions below the third layers. Moreover, the pattern

calculated using only the adatoms (topmost surface atoms) can reproduce the experiment. We found that the contribution of the topmost surface atoms to the total reflection pattern is remarkable. The RHEPD pattern enables us to determine the atomic configuration of the topmost surface layer with little influence of the underlying layers.

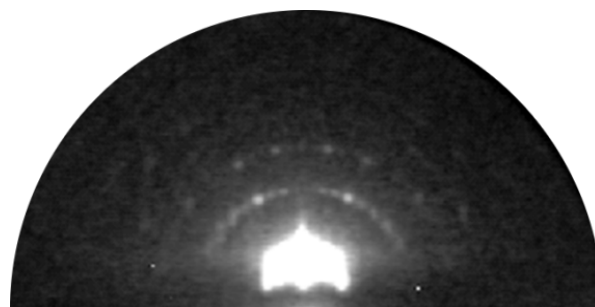


Fig. 1: Total reflection positron diffraction (TRPD) pattern from the Si(111)-7×7 surface. The glancing angle and the incident azimuth correspond to 1.3° and  $[11\bar{2}]$  direction, respectively. The incident positron energy was set at 10 keV.

### References

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