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Structural study of the Si(111)-6×1(3×1)-Ag Surface by x-ray crystal truncation rod scattering

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Introduction

The Si(111)-6×1-Ag surface is the superstructure induced by submonolayer of silver atoms. This surface has many interesting features. The surface, which takes the 6×1 periodicity at room temperature, changes to the 3×1 periodicity above 500K[1]. Moreover, it was found by low energy electron diffraction (LEED) observation that the surface takes the c(12×2) structure below 100K[2].

Another aspect is the one-dimensional structure of surface atoms. It was found by LEED and photoelectron spectroscopy that the 3×1 surfaces produced by Ag or alkali-metals are quite similar in their structures. Thus it is reasonable to apply the structure models, which were proposed for the 3×1 structure induced by alkali-metals on Si(111) surface, to the 6×1 structure. According to most of the structure models, the surface Ag atoms make one-dimensional rows. This fact expects us that the surface has one-dimensional properties.

For understanding the properties of the surface, the precise information about the arrangement of the surface atoms is necessary. In this study, the surface structure was analyzed using crystal truncation rod (CTR) scattering. In particular, the intensities along 00 rod enables us to understand the electron density perpendicular to the surface. Thus we characterized the vertical position of surface atoms and discussed about the surface structure.

Experiment and Discussion

The experiment was performed at BL15B$_2$ in which a six-circle diffractometer with a vacuum chamber is installed. The sample was prepared in the chamber, and the in-situ diffraction measurements were performed along 00 rod to obtain the information about the electron density perpendicular to the surface. The wavelength was tuned at 0.86Åand 1.2Å.

The observed intensities along 00 rod are shown in Fig. 1. The reciprocal lattice points of l=3 and 9 are identical to the 111 and 333 Bragg points in Mirror indices. Around these Bragg points, the intensities show strong asymmetry. This fact is explained by the interference between the scattering from the surface atoms and the one from the substrate.

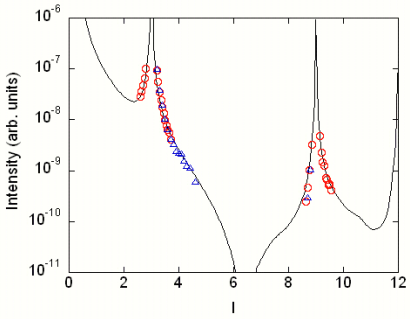

Fig.1 Intensity along 00 rod from the Si(111)-6×1-Ag surface. Red open circles and blue open triangles indicate the intensities with the wavelength of 0.86A and 1.2A, respectively. Solid line is the calculated intensity on assumption of HCC model.

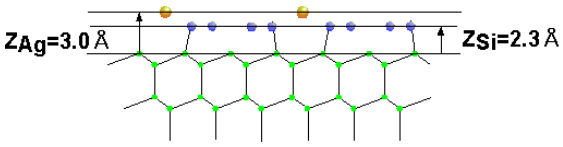

Fig.2 Structure determined by least-squares fitting analyses.

Least-squares fitting analyses were applied for the determination of the atomic arrangement perpendicular to the surface. As a result, the best-fitted model shown in Fig. 2 was obtained. The heights of the Ag and Si atoms were determined at 3.04 ± 0.01Å and 2.31 ± 0.01Å, respectively. The structure agrees well with the honeycomb-chain-channel (HCC) model proposed for the 3×1 structure induced by alkali-metals[3].

It is interesting to compare the 6×1 structure with Si(111)-√3×√3-Ag surface. The heights of both Ag and reconstructed Si atoms are quite similar in two surfaces. The positions of surface atoms do not change during the desorption of Ag atoms.

References

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