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Development of a Manipulator for Surface X-ray Diffraction at Low Temperature and Investigation of Si(111)-6x1-Ag Surface

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Introduction

Semiconductor surface is a good example for studying low-dimensional physics. Especially, the phase transition of surface superstructure at low temperature has received much attention in recent years. Even they have studied by many techniques such as LEED, RHEED, STM, photoelectron spectroscopy, however, few surface structure including the top layer of the substrate is well known.

Surface x-ray diffraction is a powerful tool to investigate the arrangement of atoms not only for three-dimensional crystals, but also for surface superstructures. In this work we developed a manipulator that is able to cool down the sample to about 70K and is suitable for the measurement of crystal truncation rod (CTR) scattering. From CTR scattering intensities, the relative position of the surface atoms against the substrate can be obtained. The manipulator is combined with the six-circle diffractometer equipped in the beamline BL15B2.

By using the manipulator, we analyzed the structure of Si(111)-6×1-Ag surface. The Si(111)-6×1-Ag surface, composed of 1/3 ML of Ag on Si(111) surface, has some unique properties. One of the uniqueness is the arrangement of the surface atoms. Structure models hitherto proposed for the surface structure have a common feature that Ag atoms make one-dimensional chains. Thus it is predicted that the surface has one-dimensional properties. The structure of the surface also shows dramatic temperature dependence. The surface, which has 6×1 periodicity at room temperature, changes to a 3×1 structure at temperature higher than 220 °C. Moreover, recent LEED and photoelectron spectroscopy studies revealed that the surface takes a c(12×2) structure at 100K[1].

Experiment and Discussion

The experiment was performed at BL15B2 in which a six-circle diffractometer with a vacuum chamber is established. The sample was prepared as follows. First, a Si(111) wafer in the vacuum chamber was heated at 1250 °C by direct current heating and we obtained the clean structure. Next, 1ML of Ag was deposited on the surface to make the Si(111)-$\sqrt{3}\times\sqrt{3}$ -Ag structure. Finally, the sample was heated to about 600 °C for desorption of the surface Ag atoms and we obtained the 6×1 structure.

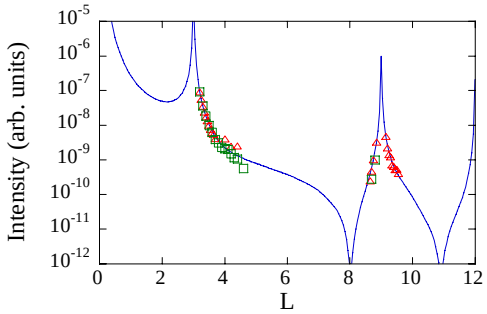

Fig.1 Intensity along 00 rod from Si(111)-6×1-Ag surface. Open triangles and open squares indicate the intensities with the wavelength of 0.86A and 1.2A, respectively. Solid line is the calculated intensity on assumption of Collazo-Davila model.

A RHEED pattern observed after the desorption showed the bright 6×1 pattern with three-fold symmetry.

The in-situ diffraction measurement was performed along 00 rod to obtain the information about the electron density perpendicular to the surface. The wavelength was selected at 0.86 Å and 1.2 Å. Figure 1 shows the intensity variations along 00 rod. Asymmetric profile around 333 Bragg reflection (L=9) is clearly seen, that is because of the interference between the scattering wave from the surface atoms and the one from the substrate. From the analysis using a least-squares fitting, the height of the Ag atoms relative to the substrate will be obtained. On the other hand, the data is not enough for determining the structure of the Si layers under the surface Ag layer because of the lack of the information at the weak intensity region between the Bragg points.

References

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