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Structural study of the Si(111)-5×2-Au surface by surface X-ray diffraction

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Introduction

Metal-induced structures on semiconductor surface have been frequently studied because of their unusual physical properties and their potential use in nano-electronic devices. We have studied the Si(111)-5×2-Au surface, which is one of various phases induced by minute amounts of Au deposited on the clean Si(111) surface and is a self-organized one-dimensional Au chain along the [-110] direction. It was first discovered about 30 years ago and has been investigated using many experimental techniques since then. However, there is no consensus on the atomic geometry in this surface structure. In this study we carried out surface X-ray diffraction experiments to determine the structure precisely.

Experimental

Our experiments were performed at beamline 15B2 of the Photon Factory, where a six-circle X-ray diffractometer with an ultrahigh vacuum (UHV) chamber is installed. Sample fabrication was performed in UHV (base pressure was 5×10^{-10} Torr). First we obtained a clean Si(111)-7×7 surface by resistive heating of the sample to 1200°C. Then 0.4 ML Au was deposited on the surface, which was kept at 630°C, to make the Si(111)-5×2-Au structure. The surface superstructure was confirmed by RHEED.

The two-dimensional atomic geometry was investigated by grazing incidence X-ray diffraction (GIXRD). The experiment was conducted at room temperature. The wavelength was 0.86 Å, the incidence angle was 0.5° and in-plane intensities were measured at L=0.2 (L=3 corresponds to the 111 Bragg reflection).

Results and Discussion

In the GIXRD experiment, we observed 67 symmetry-independent in-plane fractional-order reflections. In the analysis, we first calculated the Patterson function, which is the Fourier transform of the structure factors. Fig. 1 (a) shows a contour map of the Patterson function calculated from the experimental data. The peaks in the Patterson map indicate interatomic vectors of the surface structure in real space. The interatomic vectors extracted from Patterson map are consistent with previously proposed models for the Si(111)-5×2-Au structure. It was, however, not possible to differentiate between the different proposed models by the Patterson map alone.

Then we refined the atomic positions. In the calculation, six Si atoms and four Au atoms in the primitive unit cell were considered. The coordinates were varied to reproduce the measurement results. The results of fitting the Au positions are compared with three major proposed models (Marks & Plass model [1], Erwin model [2] and Riikonen model [3]) in Fig. 1 (b). The structural model proposed by Erwin [2] agrees best with our experimental results. In this model each unit cell contains two honeycomb chains: one honeycomb chain is formed from hexagons of alternating Au and Si atoms, and one from hexagons of only Si atoms.

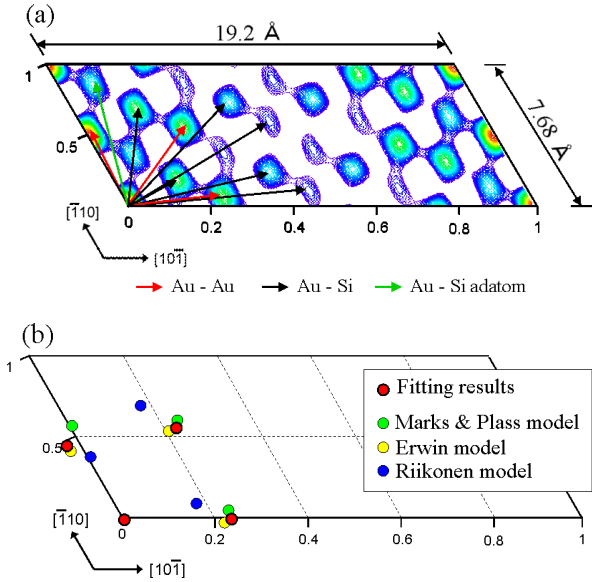

Fig. 1 (a) Contour plot of the Patterson function in the primitive 5×2 unit cell. Each arrow indicates interatomic vectors in real space. (b) Au positions derived from fitting to the experimental data (red circles) and those of three structural models (green, yellow and blue circles).

References

[1] L.D. Marks, R. Plass, Phys. Rev. Lett. 75, 2172 (1995)
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