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Structural analysis of Si(1 1 1)–$\sqrt{21} \times \sqrt{21}$-Ag surface by reflection high-energy positron diffraction

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Abstract

The atomic structure of Si(1 1 1)–$\sqrt{21} \times \sqrt{21}$-Ag surface, which is formed by the adsorption of small amount of Ag atoms on the Si(1 1 1)–$\sqrt{3} \times \sqrt{3}$-Ag surface, was determined by using reflection high-energy positron diffraction. The rocking curve measured from the Si(1 1 1)–$\sqrt{21} \times \sqrt{21}$-Ag surface was analyzed by means of the intensity calculations based on the dynamical diffraction theory. The adatom height of the extra Ag atoms from the underlying Ag layer was determined to be 0.53 Å with a coverage of 0.14 ML, which corresponds to three atoms in the $\sqrt{21} \times \sqrt{21}$ unit cell. From the pattern analyses, the most appropriate adsorption sites of the extra Ag atoms were proposed.

Keywords: Surface structure; Reflection high-energy positron diffraction (RHEPD); Total reflection; Silicon; Silver

1. Introduction

In 1994, it has been found that a $\sqrt{21} \times \sqrt{21}$ super-lattice structure is induced by adsorption of Au adatoms on a Si(1 1 1)–$\sqrt{3} \times \sqrt{3}$-Ag surface [1,2]. Similar $\sqrt{21} \times \sqrt{21}$ periodicity was also observed by the adsorption of noble metal atoms such as Ag and Cu [3–5] and alkali metal atoms such as Na, K, and Cs [6–8]. The atomic configurations of the $\sqrt{21}$ structure family are considered to be the same because of similarity of the electronic structure. Furthermore, the $\sqrt{21} \times \sqrt{21}$-Ag surface shows a drastic increase in the electrical conductivity as compared to the Si(1 1 1)–$\sqrt{3} \times \sqrt{3}$-Ag surface [9]. Recently, the mappings of the Fermi surfaces have been performed to investigate the origin of the high electrical conductivity and make clear the mechanism of the doping with respect to the adsorption on the Si(1 1 1)–$\sqrt{3} \times \sqrt{3}$-Ag surface [10,11]. Because of importance as a prototypical two dimensional metal system, the adsorption on the Si(1 1 1)–$\sqrt{3} \times \sqrt{3}$-Ag surface attracts much attention. So far, the structure analyses were carried out by using the scanning tunneling microscopy (STM) [1,2,12] and surface X-ray diffraction (SXRD) [13]. However, the several kinds of structure models have been proposed and hence opinions are divided on this matter.

Nogami et al. proposed the structure model, where all the additional Au atoms sit on the center of Ag triangles of the original Si(1 1 1)–$\sqrt{3} \times \sqrt{3}$-Ag surface [1]. In Nogami's model, five Au atoms are included in the unit cell of the $\sqrt{21} \times \sqrt{21}$ super-lattice structure. Ichmiya et al. proposed that the Au atoms are situated at the center of the Si trimer [2]. The number of the Au atoms in Ichimiya's model is three. Tong et al. proposed another structure model, which resembles to the Nogami's model although the number of the additional atoms is four [12]. These models were built on the STM observations. Using the SXRD method, Tajiri et al. proposed the new model where the four Au atoms relatively aggregate to each other and one atom is apparent from them [13]. Tong et al. demonstrated that the honeycomb chained triangle (HCT) or

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inequivalent triangle (IET) structure of the original Si(1 1 1)–$\sqrt{3}\times\sqrt{3}$-Ag was preserved for the Si(1 1 1)–$\sqrt{21}\times\sqrt{21}$-Ag surface using the angle-resolved photoemission spectroscopy (ARPES) [14] and the core-level photoemission [15]. It should be noticed that the element of the adsorption atom is Ag for Tong model and is Au for the other models.

In this paper, we investigated the optimum adsorption site of the additional Ag atoms for the Si(1 1 1)–$\sqrt{21}\times\sqrt{21}$-Ag surface using the reflection high-energy positron diffraction (RHEPD). The RHEPD is a newly powerful tool to study the surface structure, especially, the topmost atomic positions [16,17]. The remarkable advantage using the RHEPD for the surface science study is that the total reflection occurs at the grazing incidence. In the total reflection region, the incident positron beam is not able to penetrate the bulk and hence the diffracted intensities include the information about only the topmost surface atoms. Analyzing the totally reflected intensities, we can accurately determine the atomic positions and the thermal vibrational amplitudes with respect to the topmost surface layer [18,19]. In this study, we measured the RHEPD rocking curves from the Si(1 1 1)–$\sqrt{21}\times\sqrt{21}$-Ag surface. From the intensity analysis based on the dynamical diffraction theory, we determined the optimum surface structure. To obtain the consensus, we also performed the RHEPD pattern analysis. We will show a new structure model suitable for the Si(1 1 1)–$\sqrt{21}\times\sqrt{21}$-Ag surface structure.

2. Experimental procedure

Samples with a dimension of $15\times5\times0.5\ \mathrm{mm}^3$ were cut from a *n*-type mirror-polished Si(1 1 1) wafer (resistivity: 1–10 Ω cm). These were flushed at 1470 K in 10 s a few times, followed by degassing at 600 K for several hours. After the cleaning, sharp 7×7 spots were confirmed by a reflection high-energy electron diffraction (RHEED). To produce a Si(1 1 1)–$\sqrt{3}\times\sqrt{3}$-Ag structure, one monolayer (ML) of Ag atoms were deposited on a Si(1 1 1)-7×7 surface kept at 770 K using a electron beam evaporator, where 1 ML corresponds to $7.83\times10^{14}\ \mathrm{cm}^{-2}$. Subsequently, the sample was cooled down to 110 K using liquid nitrogen. Additional deposition of Ag atoms was done on the Si(1 1 1)–$\sqrt{3}\times\sqrt{3}$-Ag surface at low temperature. The deposition was stopped when the $\sqrt{21}\times\sqrt{21}$ spot intensities by RHEED reached the maximum. The deposition amount was expected to be 0.14 ML from the evaporation rate.

The experiments were carried out in a ultra-high vacuum chamber equipped with a positron source of ^{22}Na and magnetic lens system [20]. The positron beam energy was set at 10 keV. In the measurement of rocking curves, the glancing angle (θ) was varied up to 5.9° at a step of 0.1° with the rotation of a sample holder. The RHEPD pattern was taken with a multi-channel plate and charge coupled device camera. The image of the pattern was installed in a personal computer. The temperature of the sample was measured using a thermocouple attached at the sample holder.

3. Results and discussion

Fig. 1(a) and (b) show the RHEPD patterns measured from the Si(1 1 1)–$\sqrt{3}\times\sqrt{3}$-Ag and Si(1 1 1)–$\sqrt{21}\times\sqrt{21}$-Ag surfaces, respectively. It should be noted that the RHEPD patterns displayed here are superposition of the left and right parts. When depositing the additional Ag atoms on the Si(1 1 1)–$\sqrt{3}\times\sqrt{3}$-Ag surface, the fractional-order spots accompanied with the Si(1 1 1)–$\sqrt{21}\times\sqrt{21}$-Ag surface appear in the higher order Laue zone. Especially, the (20/21 17/21) spots are clearly seen in the RHEPD pattern. Accordingly, the RHEPD intensities for the (1/3 1/3), (2/3 2/3) and their equivalent spots

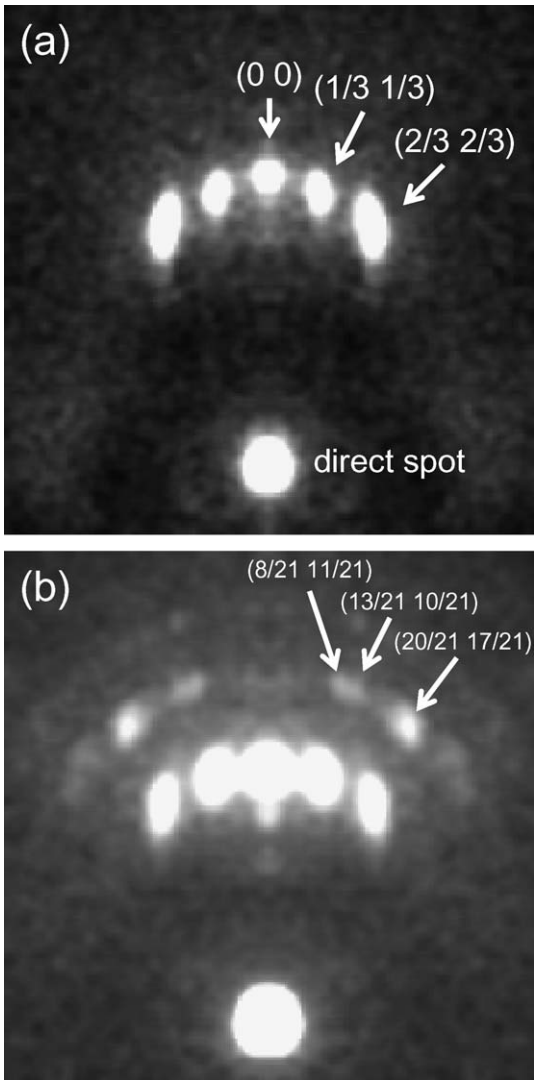

Fig. 1. RHEPD patterns observed from (a) the Si(1 1 1)–$\sqrt{3}\times\sqrt{3}$-Ag surface at $\theta=3.2°$ and (b) Si(1 1 1)–$\sqrt{21}\times\sqrt{21}$-Ag surface at $\theta=2.7°$. The incident azimuth corresponds to the [1 1 $\bar{2}$] direction. The substrate temperature is 110 K.