Structural Study of Si(111)$\sqrt{21}\times\sqrt{21}$-(Ag+Au) surface by X-ray Diffraction

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Introduction

It has been reported that surface superstructures with the $\sqrt{21}\times\sqrt{21}$ periodicity emerge by depositing noble metals (Au, Ag, or Cu) onto the Si(111) $\sqrt{3}\times\sqrt{3}$-Ag (the$\sqrt{3}$-Ag) surface[1-3]. Recently very high surface electrical conductances due to the surface-state bands have been reported for these $\sqrt{21}\times\sqrt{21}$ surfaces. Thus the atomic arrangements of these $\sqrt{21}\times\sqrt{21}$ surfaces are of great interest. In this work, we study the structure of the Si(111) $\sqrt{21}\times\sqrt{21}$-(Ag + Au) surface by grazing incidence X-ray diffraction.

Experimental and Result

The experiment was carried out by using the six-circle surface X-ray diffractometer with an ultra-high vacuum (UHV) chamber installed in the beamline 15B2 of the Photon Factory[4]. Two Knudsen cells were used for evaporation of Ag and Au.

A total of 84 in-plane integrated intensities were collected, in which 72 reflections were inequivalent. These were all fractional order reflections peculiar to the $\sqrt{21}\times\sqrt{21}$ periodicity. Though the reflections coming from the $\sqrt{3}\times\sqrt{3}$ periodicity were also observed, they were not used in the present analysis.

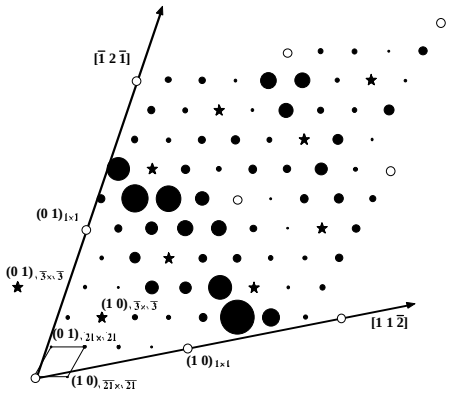

Fig.1. Diffracted intensities from the Si(111) $\sqrt{21}\times\sqrt{21}$ (Ag+Au) by GIXD.

Figure 1 shows the reciprocal space map concerned with the observed structure factor intensities. Open circles, asterisks and filled circles correspond to the in-plane reciprocal lattice points of the 1x1, $\sqrt{3}\times\sqrt{3}$, and $\sqrt{21}\times\sqrt{21}$ periodicities, respectively. The filled circles are drawn so that the areas are proportional to the observed structure factor intensities.

First, we calculated the contour map of the Patterson function to find interatomic vectors. Then we made least squares fits for a number of models which are consistent with the Patterson map. The fitting results for the structural models that contain only Au adatoms gave high $\chi 2$ values. This indicates that the Ag triangle and the Si trimer displace from the $\sqrt{3}\times\sqrt{3}$ framework[5] considerably.

Finally we could find out four models that are consistent with the experimental results on the assumption that Au adatoms sit on the centers of Ag tringles, two of which are shown in Fig.2.

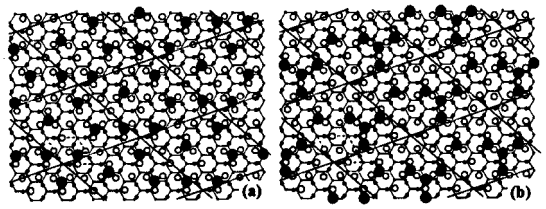

Fig.2. Two of four models proposed for the Si(111)$\sqrt{21}\times\sqrt{21}$-(Ag+Au) surface. Lines show the $\sqrt{21}\times\sqrt{21}$ unit cell. Filled large circles and open circles mean Au and Ag atoms.

Conclusion

The model proposed by Tong et al.[3] and Ichimiya et al.[2] are ruled out from the results found in this work. The model proposed by Nogami et al.[1] that contains five Au adatoms is most preferred in the three models. Three other models with five Au adatoms are also favored if Au adatoms sit upon the centers of Ag triangles. It was found that one of the three other models, shown in Fi2(b), can explain well the STM images obtained by Nogami et al.[1] as well. The brightest spot is assigned as the clusters of four Au adatoms, and the triangle images locating around the origin of the $\sqrt{21}\times\sqrt{21}$ unit cell as the images of IET model[6], and the rest one as a Au adatom. In any models, underlying structure of the Ag triangle and Si trimers displaces from the $\sqrt{3}\times\sqrt{3}$ framework considerably[7].

References

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