Temperature dependence of the Si(111)-$\sqrt{3}\times\sqrt{3}$-Ag structure

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Introduction

The structure of Si(111)- $\sqrt{3}\times\sqrt{3}$-Ag had been in controversy for years until a honeycomb chained triangle (HCT) model was proposed[1]. Since then, the HCT model has been supported by various kinds of surface science techniques. Recently, however, a new model called inequivalent triangle (IET) model has been proposed by first-principles calculations[2] and STM studies at low temperatures[3]. Thus the IET model casts doubts on the HCT model. For this reason, we study temperature dependence of the Si(111)-$\sqrt{3}\times\sqrt{3}$-Ag structures, and discuss the phase transition of the surface in this report.

Figure 1(a) and 1(b) show the HCT and IET models. The IET model is characterized as a structure in which a large Ag triangle indicated dashed lines in the HCT model is rotated around its center by about 6 degrees. As a result, the IET model, losing a mirror line, has a lower symmetry in comparison with the HCT model.

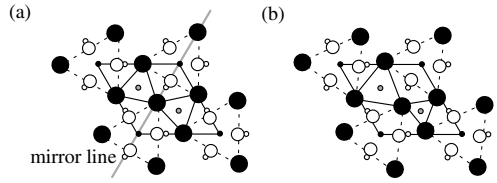

Fig.1. A honeycomb chained triangle (HCT) model(a) and an inequivalent triangle (ITE) model(b).

Experimental results and discussions

Experiments using grazing incidence X-ray diffraction were performed at BL-15B2. Figure 2(a) and 2(b) show Patterson maps calculated from intensity distributions obtained at RT and LT(50K). A single peak indicated A in Fig.2(a) splits into two peaks, A1 and A2, in Fig.2(b). This means that Ag atoms take the HCT structure at RT and they change into the IET structures at LT. Two peaks correspond to two domains in a relation of surface twins in which Ag triangles are rotated in opposite directions. Detailed analysis of the least squares fit also showed the same results for both data where anisotropic Debye-Waller factors were used. Ag atoms making triangles are found to be vibrating mainly in the rotational directions, particularly at RT.

Next we observed temperature dependence of some diffraction spots from RT to 50K. At low temperatures diffuse scattering due to surface twins is observed. From temperature dependence of the integrated intensities of diffuse scattering, it was found that the phase transition temperature is about 150K , and the critical exponent beta takes a large value of 0.27. We also analyzed temperature dependence of the integrated intensities of Bragg components. Their intensities changed at the phase transition temperature.

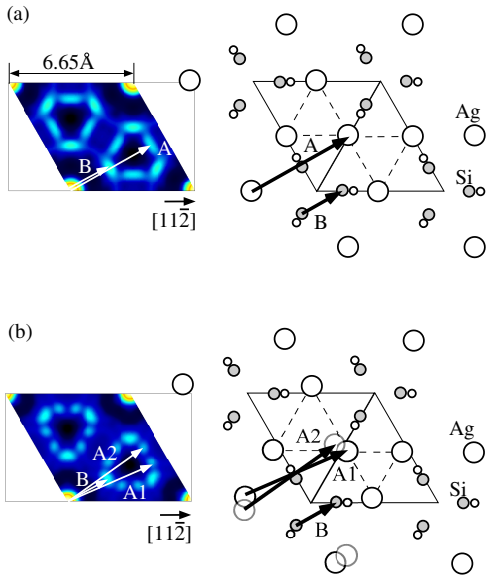

Fig.2. Patterson maps calculated from the integrated Bragg intensities of diffraction spots observed at room temperature (a) and a low temperature of 50K(b).

In summary, the structure of Si(111)-$\sqrt{3}\times\sqrt{3}$-Ag was determined to be the HCT structure with strong anisotropic thermal vibrations at RT and the IET structure with surface twins at LT. The phase temperature and critical exponent of the surface were determined. Order-disorder phase transitions are not favored; honeycomb protrusions observed in STM images at RT are not interpreted as thermal fluctuations between twin states. The present work rather supports a displacive type phase transition.

References

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