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Thermal Vibration of surface atoms on Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag

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Introduction

The structure of Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface has attracted renewed interests in recent years. The arrangement of surface atoms has been thought to be a HCT (honeycomb-chained triangle) structure proposed from surface x-ray diffraction measurements[1]. However, recent first-principle calculations suggested that an IET (inequivalent triangle) structure is more stable than the HCT structure[2]. Moreover, STM images obtained at low temperature showed twin domains which support the IET structure[3]. Thus the surface has been studied by many scientists from a viewpoint of phase transition. It is also the target of investigation which structure is correct at room temperature.

In previous work we studied the structures of Si(111)-$\sqrt{3}\times\sqrt{3}$ -Ag surface at low temperature (50K) and room temperature using surface x-ray diffraction[4]. As a result, the intensities at the low temperature supported IET model, while the intensities at room temperature was well explained by HCT model. In this report we make more detailed analysis of the thermal vibration of surface atoms in the high temperature phase.

Results and discussions

Measurements were performed at BL-15B$_2$ using a six-axis diffractometer with a vacuum chamber. GIXD (Grazing incidence X-ray diffraction) was used for analyzing the in-plane arrangement of surface atoms. Figure 1 shows the arrangement and thermal vibrations of surface atoms determined by least-squares refinement of the intensity distribution. Ellipses display anisotropic feature of the vibration. The surface Ag atoms strongly oscillate along the direction that triangles of Ag atoms rotate around their centers. This direction is the same that found in the structural change from the HCT structure to the IET structure. The displacement from equilibrium positions is also close to the difference in atomic positions of Ag atoms between the IET and HCT structures.

Figure 2 shows temperature dependence of the displacement of Ag atoms in the radial(U_{11}) and rotational(U_{22}) directions, respectively. The displacement at 0K, extrapolated from line fitting, does not fall down to zero value. This means that the assumption of anisotropic harmonic oscillation is not enough for describing the thermal vibration of surface atoms.

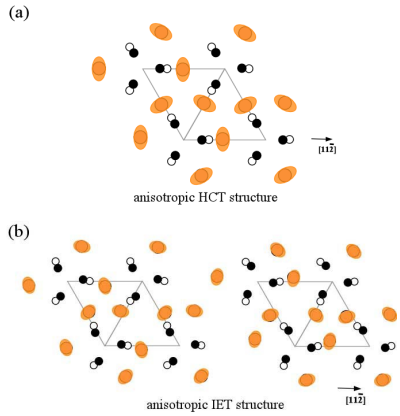

Fig.1 Schematic view of thermal vibrations of surface Ag atoms, (a) at room temperature, (b) at low temperature.

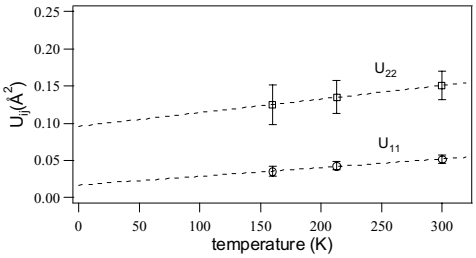

Fig.2 Temperature dependence of thermal vibrations of surface atoms in the radial and rotational directions.

In summary, we investigated the thermal vibration of surface atoms using surface x-ray diffraction. For more precise description of thermal vibrations, we should analyze the structure by taking into account anharmonicity in thermal vibrations. This leads us to a better understanding of the structure and phase transition. We are collecting the intensities at high temperatures for this purpose.

References

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