Structure analysis of Sb/Bi heterostructure on Si(111) by Total-Reflect High-Energy Positron Diffraction with 2DMAT

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Introduction

Since the experimental demonstration of topological insulators, they have actively been investigated due to their intriguing fundamental properties and potential applications in spintronics devices and quantum computations. Recently a lot of studies focusing on topological phase transitions have been performed in various materials, and topological phase transitions by epitaxial strain at the interface are very useful from the viewpoint of applications because they do not require any external field environment and are compatible with surface sensitive experimental technique.

Group-V semimetal bismuth (Bi) and antimony (Sb) turn from being topologically trivial to nontrivial by slight lattice strain. For Bi, the phase transition to a topological semimetal induced by 0.4%–1% lattice strain has theoretically been predicted [1]. Various theoretical predictions have also been reported for ultrathin Sb films. For instance, freestanding Sb(111) films with less than 4 BL have been reported to be topologically trivial, however several calculations predicted that the topological phase transition can be induced by tuning structural parameters [2]. To observe and discuss the details of the topological phase transition in Sb ultrathin films experimentally, it is necessary to fabricate Sb thin films on substrates with a larger lattice constant and to analysis and determine the atomic structure.

In this work, we have performed structure analysis of ultrathin Sb films on Bi(111) using by total-reflect high-energy positron diffraction (TRHEPD). A structural analysis of Bi was carried out first, followed by a stacked Sb structure. The TRHEPD experiment consists of measuring a series of the diffraction patterns for a fixed incident azimuthal direction at various glancing angles θ. Here, the rocking curve is defined as the diffraction intensity of the (00) spot plotted as a function of θ. In the structural analysis, the experimental rocking curves are compared with those calculated for various structural models. For analysis, calculations of the rocking curves for TRHEPD were performed by the structure-analysis program 2DMAT [3].

Results and discussion

Figure 1(a) shows the rocking curves of Bi(111) thin film for 10BL measured under the many-beam (MB) condition. In the MB condition, the beam is incident along a symmetric direction, thus the rocking curve in the MB condition essentially gives the information on the atomic positions in the in-plane and out-of-plane direction. Here, we considered a structural model with the Bi interlayer distance and the in-plane lattice constant as parameters. The results of the analysis showed that the structure shown in Fig. 1(b) reproduced the experimental results best; the in-plane lattice constant is 4.38 Å, and the

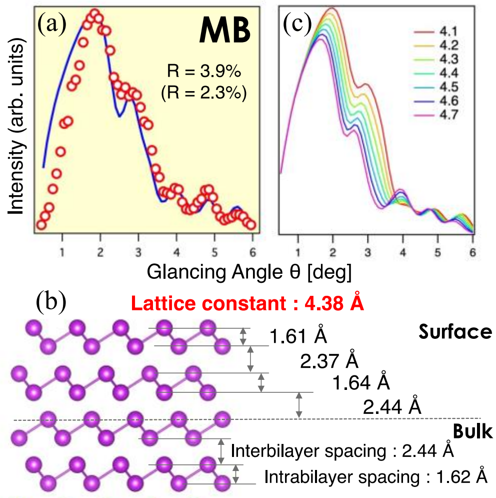

Fig. 1: Experimental measured rocking curves under MB condition for Bi thin films (10 BL) with calculated curves with the structure model in (b). (c) Dependence of the rocking curve on the in-plane lattice constant.

layer distances correspond well with the results of previous studies. We also calculated rocking curves under the OB condition with several in-plane lattice constant [Fig. 1(c)]. One sees the shape of the rocking curve changed significantly in response to the value of the in-plane lattice constant, and we found the experimental results are not reproduced by the lattice constant of bulk Bi (4.54 Å). This result suggest that the Bi is a topologically non-trivial.

Next we have performed structure analysis of ultrathin Sb films (2 BL) on Bi(111). By electron diffraction, we have confirmed that Sb thin film grows on Bi with different lattice constant. However, no moiré pattern was observed in electron diffraction, so it is not possible to construct a structural model assuming a long-period structure. Therefore we have performed TRHEPD measurement under the one-beam (OB) condition. In the OB condition the beam

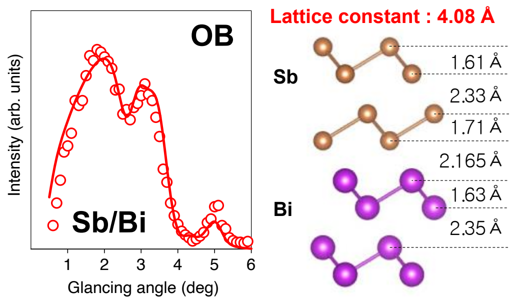

Fig. 2: (Left) Experimental measured rocking curves under OB condition and (right) determined structure model for Sb/Bi heterostructure.

is incident along an off-symmetric direction. The Rocking curve in the OB condition essentially gives the information on the atomic positions in the out-of-plane direction and atomic density in layer. In this analysis, the lattice constant of Sb relative to Bi 1 BL was estimated by calculating the density of Sb. Figure 2 shows the rocking curves of Sb/Bi heterostructure measured by TRHEPD and determined structure model. As a result of the analysis, the in-plane lattice constant of Sb thin films on Bi was estimated to be 4.08 Å. This value corresponds with that estimated from electron diffraction. For more detailed structure determination, a heterostructure model will be constructed from this estimate in the future, and the structure will be analyzed in a giant lattice system.

References

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