Structure analysis of atomic layer alloy with Rashba effect studied by TRHEPD

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Introduction

The superconducting phenomenon that occurs in the spin-split electronic state due to the Rashba effect is theoretically predicted to be an unconventional superconducting state where *s*-wave and *p*-wave superconductivity coexist (Rashba-SC). In order to investigate the details of this Rashba-SC, material exploration and research on its electronic states are being actively conducted. Previous studies have shown that (Bi, Pb) single-atom layer (SAL) alloys on Ge(111) and Si(111) substrates are predicted to exhibit Rashba-type spin-split bands due to the strong spin-orbit coupling of Pb and Bi [1]. We revealed several metallic electronic states exhibit with spin-splitting in the (Bi, Pb)-Ge(111)-2×2 structure by angle- and spin-resolved photoemission spectroscopy.

In this study, we performed structural analysis of several SAL structures exhibiting the Rashba effect in order to discuss the details of the Rashba effect in SAL structures from a structural perspective, using by total-reflect high-energy positron diffraction (TRHEPD). Here, we report mainly on structural analysis of Bi/Ge(111), Pb/Ge(111), and (Bi, Pb)/Ge(111).

Experiments and analysis methods

The TRHEPD measurements were performed at the Slow Positron Facility, KEK. The TRHEPD experiment involves measuring a series of diffraction patterns for a fixed incident azimuthal direction at various glancing angles (θ). In this context, the rocking curve (RC) 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. The locking curves for each structure were calculated and compared with experimental results using the structural analysis program ODAT-SE (2DMAT) [2]. Specifically, large-scale calculations were performed on supercomputers, including: (i) long-period structure induced by the striped-incommensurate (SIC) phase in Pb/Ge(111), and (ii) structural analysis with multiple parameters set for (Bi, Pb) SAL structure with unclear structural model.

Results and discussion

Figure 1(a) shows the results of structural analysis for Pb/Ge(111)-√3×√3 structure. The RC calculated from the structural model proposed by Otsubo *et al*. [3] reproduced the experimental results relatively well. In this study, structural optimization was performed using Nelder-Mead method, and we concluded that the structural model shown in Fig. 1(a) is the most reliable. Additionally, rocking curves were

calculated for a long-period structure incorporating the SIC phase, which revealed that there were no significant changes in the calculation results. Structural analysis was also performed on Bi/Ge(111)- √3×√3 structure, as shown in Fig. 1(b). The RC calculated from the structural model proposed in previous study [4] reproduced the experimental results very well. In both structures, it was found that there was almost no structural relaxation of Ge in the out-of-plane direction. Furthermore, we also found that slight differences in the in-plane positions of Pb (T_4 site) and Bi (T_1 site) atoms greatly affect the shape of RC.

Figure 2 shows the RCs of (Bi, Pb)/Ge(111)-2×2 structure and the RCs calculated from the structural model proposed in previous studies. The calculated RC from the 2×2 structure model proposed by Mihalyuk *et al*. [1] does not match the experimental RC. Currently, we are performing structural analysis following two different approaches. The first approach is structural optimization based on the Mihalyuk model. In this approach, the structure can be determined by varying the distances and configurations between atoms. The second proposal addresses the fact that the ratio of Bi and Pb in the 2×2 unit cell has not yet been determined. To investigate this, we will investigate structural models by adjusting the atomic densities of Pb and Bi as parameters.

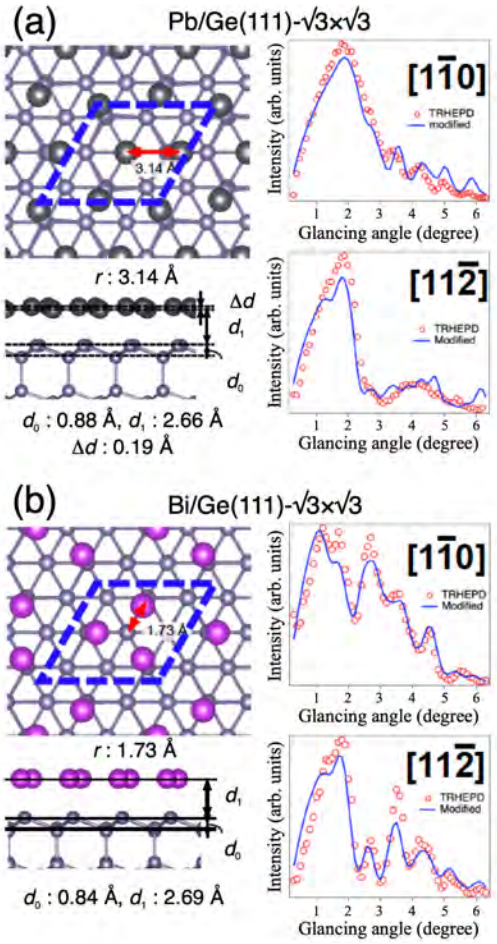

Fig. 1: Results of structural analysis by TRHEPD of (a) Pb/Ge(111)-√3×√3 and (b) Bi/Ge(111)-√3×√3. (left) Determined structural model. (right) RCs with calculated curves under many-beam conditions.

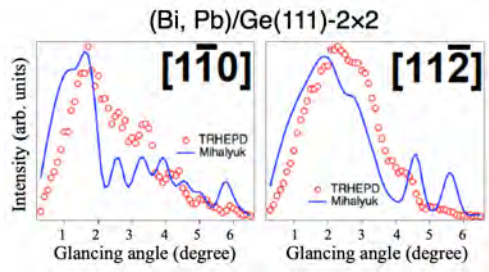

Fig. 2: RCs under many-beam conditions for (Bi, Pb)/Ge(111)-2×2 structure with calculated curves from proposed structural model in previous study [1].

References

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