SPF/2010G652

Structure analysis of Ag_2Pb surface alloy by KEK-RHEPD

Yuki Fukaya[1,*], Iwao Matsuda[2], Masaki Maekawa[1], Izumi Mochizuki[1], Ken Wada[3], Toshio Hyodo[3], and Atsuo Kawasuso[1],
[1]JAEA, Takasaki 370-1292, Japan
[2]University of Tokyo, Chiba 277-8581, Japan
[3]KEK-IMSS, Tsukuba 305-0801, Japan

1 Introduction

By the deposition of a 1/3 monolayer (ML, 1 ML = 1.38×10^{15} cm^{-2}) of Bi or Pb atoms on the Ag(111) surface, the surface alloy phase with a $\sqrt{3}\times\sqrt{3}$ structure is formed. This surface alloy is known as a giant Rashba surface [1]. The Rashba energy for the Ag_2Bi surface alloy is estimated to be 200 meV [1], which is much larger than that for two-dimensional hetero-semiconductors (~1 meV). First-principles calculations suggested that the magnitude of the Rashba energy is closely related to the outward displacement of the topmost heavy element [2]. However, the relationship between them still remains unresolved.

Reflection high-energy positron diffraction (RHEPD) is a surface-sensitive tool to determine the topmost atomic structure and property owing to the total reflection. Recently, a new RHEPD apparatus was developed using an intense position beam from a linac at the Slow Positron Facility at the Institute of Materials Structure Science, KEK [3]. The fractional spots for the Si(111)-7×7 surface were clearly observable. In this report, measurements of the RHEPD rocking curves from the Ag_2Pb alloy surfaces with changing the film thickness of the underlying Ag layers are described. The surface structure was analyzed using the dynamical diffraction theory.

2 Experiment

To make crystalline Ag(111) thin films, Ag atoms were deposited onto the Si(111)-7×7 surface at 130 K. The substrates were cut from a mirror-polished Si(111) wafer. After gradually annealing up to room temperature, well-ordered Ag(111) thin films were formed. Subsequently, 1/3 ML Pb atoms were deposited on the Ag(111)-1×1 surface at 400 K.

The RHEPD experiments were carried out at the slow positron beam line SPF-B1 at the Slow Positron Facility, KEK [3]. The positron beam energy was 10 keV. To measure the rocking curves, the glancing angle was varied up to 6° by rotating the sample.

3 Results and Discussion

Figure 1 displays the RHEPD rocking curves of the specular spots measured for the Ag_2Pb surface alloys with Ag film thicknesses (t_{Ag}) of 6, 11, 22 ML under the one-beam condition. In this condition, the rocking curve depends mainly on the vertical displacement of the atomic positions. Although the change in the rocking curves with t_{Ag} is small, the intensitiy in the glancing angle range of 2.0°-4.5° gradually decreases as t_{Ag} increases. This indicates that the Pb atoms are shifted upward with increasing t_{Ag}.

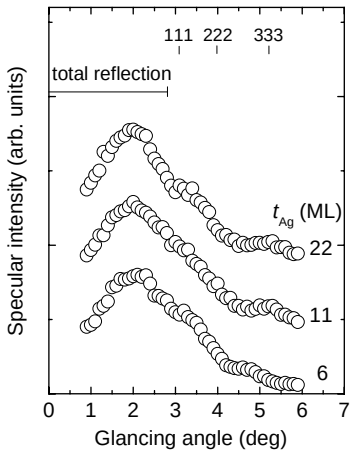

Fig. 1 (a) RHEPD rocking curves of the specular spots measured for the $\sqrt{3}\times\sqrt{3}$ of Ag_2Pb surface alloys with t_{Ag} = 6, 11, and 22 ML. The critical angle for total reflection is estimated to be 2.7°. The index of the Bragg reflection is shown at the top of figure.

To determine the outward displacement of the Pb atoms, the RHEPD intensities were calculated based on the dynamical diffraction theory. It was found that the outward displacement of the Pb atoms increases with increasing t_{Ag}. In order to confirm the displacement with t_{Ag}, the measurements of the rocking curves for the Ag_2Pb surface alloy with various t_{Ag} are needed. Further, to verify the relationship between the atomic displacement and the Rashba energy, the surface electronic band structures will be measured by using angle-resolved photoemission spectroscopy (ARPES).

References

[1] C. R. Ast *et al*., Phys. Rev. Lett. **98** (2007) 186807.
[2] G. Bihlmayer, S. Blügel, and E. V. Chulkov, B **75** (2007) 195414.
[3] K. Wada *et al*., Eur. Phys. J. D **66** (2012) 37.

* fukaya.yuki99@jaea.go.jp