Thickness Dependence of Electronic Structure of Bi Thin Films on Au(111)

N. Nishimoto [a], H. Yamaguchi [b], T. Asano [b], Y. Fujisawa [c], K. Sumida [c],
H. Sato [c], K. Miyamoto [c] and T. Okuda [c,d,e]

[a] Department of Physics, Faculty of Science, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 739-8526, Japan.
[b] Graduate School of Advanced Science and Engineering, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 739-8526, Japan.
[c] Research Institute for Synchrotron Radiation Science, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 739-8526, Japan.
[d] International Institute for Sustainability with Knotted Chiral Meta Matter (SKCM^2), Hiroshima University, 1-3-1 Kagamiyama, Hiroshima 739-8526, Japan.
[e] Research Institute for Semiconductor Engineering (RISE), Hiroshima University, 1-4-2 Kagamiyama, Higashi-Hiroshima, 739-8527, Japan.

Keywords: Spin-Orbit Coupling, Quasi-one-dimensional structure, ARPES

Bismuth (Bi) is a heavy element and has been extensively studied in solid-state physics due to its unique electronic properties arising from its strong spin-orbit coupling (SOC). In monolayer and few-layer Bi ultra-thin films, strong SOC is predicted to induce band inversion, causing a phase transition from a semi-metallic state to a two-dimensional topological insulator [1]. While it is well known that Bi forms surface alloys with giant Rashba splitting on Ag(111) and Cu(111) substrates [2,3], the growth of Bi on Au(111) exhibits a distinct behavior. Instead of alloying, Bi on Au(111) forms various complex surface structures depending on the coverage [4]. Although reported coverage values vary in the literature, it is generally accepted that a (5×5) low-temperature adsorption phase is formed below 0.6 ML, a $(\sqrt{37} \times \sqrt{37})R25.3^\circ$ structure is formed up to 0.8 ML, and a quasi-one-dimensional $(p \times \sqrt{3})$ stripe structure is formed up to 1 ML. In the thick film regime, Bi(110) is formed. Regarding the $(p \times \sqrt{3})$ structure, previous studies have proposed a long-period Moiré model in which the periodicity p evolves as 5, 8, 11, and 14 with increasing coverage [5]. In this study, we aimed to comprehensively elucidate the relationship between surface structures and electronic structures in the Bi/Au(111) system.

A clean Au(111) surface was obtained by repeated cycles of Ar-ion sputtering (1.5 kV) and annealing (1000 K). Bi deposition was performed by molecular beam epitaxy (MBE) using a Knudsen cell (K-cell) under ultra-high vacuum conditions ($\sim 10^{-8}$ Pa). We identified the surface structures by comparing experimental Low-Energy Electron Diffraction (LEED) patterns with simulations based on structural models from previous studies. Specifically, the periodicity p of the $(p \times \sqrt{3})$ structures was identified based on the relative size of the characteristic triangular patterns observed in the LEED images (Figure 1(a)-(c)). The Angle-Resolved Photoemission Spectroscopy (ARPES) measurements were carried out at HiSOR BL-7 using p-polarized light with photon energies of $h\nu = 20 \sim 70$ eV at temperatures below 100 K.

ARPES results revealed a Bi-derived surface state band (SSB) within the projected bulk band gap of Au, located near the $\overline{\mathrm{K}}$ point. We clarified that the SSB systematically shifts to larger k-values as the periodicity p increases (Figure 2(a)-(d)). Furthermore, the constant energy contour exhibits a triangular shape centered at the $\overline{\mathrm{K}}$ point. Regarding the dispersion along the k_y direction (parallel to the stripes), we revealed that it forms a characteristic band structure where electron-like and hole-like bands overlap and disperses with a variation in effective mass as k_x (perpendicular to the stripes) increases (Figure 3). In addition, we investigated the electronic states of other surface structures and compared the experimental results with band calculations. The details will be discussed in the poster presentation.

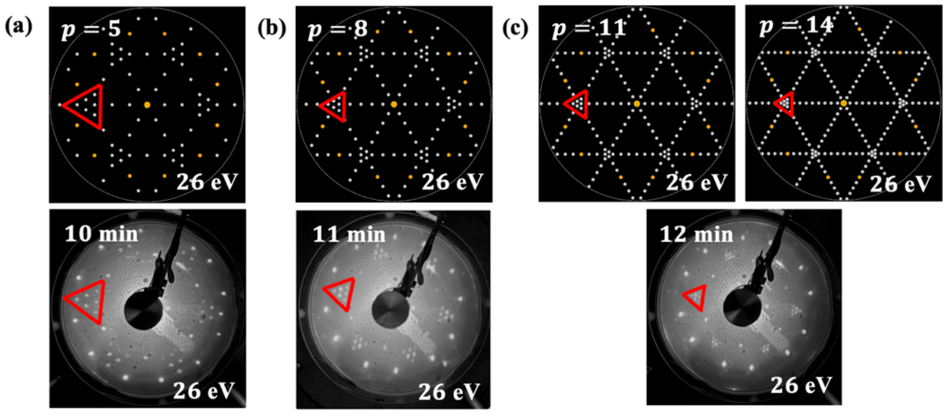

Figure 1. Comparison between experimental and simulated LEED patterns: (a) $(5 \times \sqrt{3})$; (b) $(8 \times \sqrt{3})$; (c) $(14 \times \sqrt{3})$

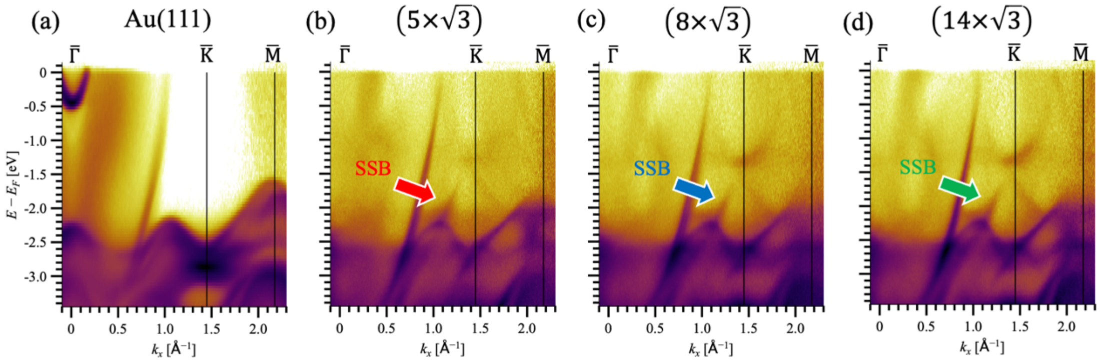

Figure 2. ARPES spectra measured at $h\nu = 44$eV along the $\bar{\Gamma} - \bar{\mathrm{K}} - \bar{\mathrm{M}}(\mathrm{Au})$ direction: (a) $(5 \times \sqrt{3})$; (b) $(8 \times \sqrt{3})$; (c) $(14 \times \sqrt{3})$

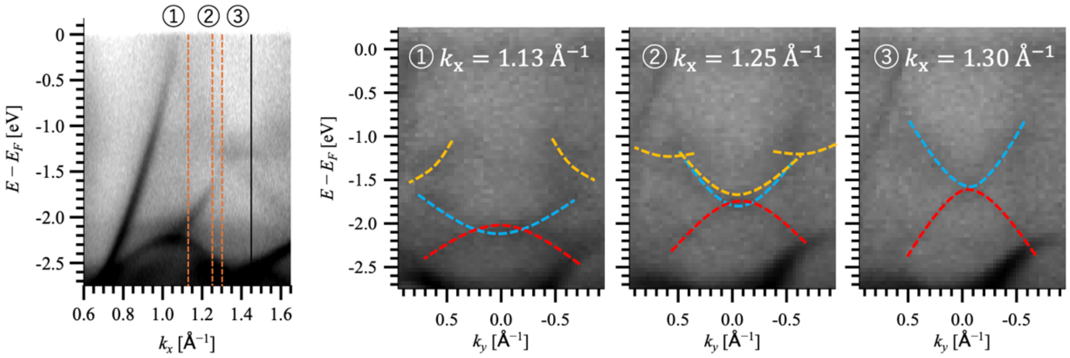

Figure 3. ARPES spectra of the $(5 \times \sqrt{3})$ structure along the k_y direction measured at the k_x positions indicated by ①–③.

REFERENCES

1. S. Murakami, Phys. Rev. Lett. **97**, 236805 (2006).
2. C. R. Ast, J. Henk, A. Ernst, L. Moreschini, M. C. Falub, D. Pacilé, P. Bruno, K. Kern, and M. Grioni, Phys. Rev. Lett. **98**, 186807 (2007).
3. H. Bentmann, T. Kuzumaki, G. Bihlmayer, S. Blügel, E. V. Chulkov, F. Reinert, and K. Sakamoto, Phys. Rev. B **84**, 115426 (2011).
4. N. Kawakami, C.-L. Lin, K. Kawahara, M. Kawai, R. Arafune, and N. Takagi, Phys. Rev. B **96**, 205402 (2017).
5. P. V. Vicente, T. Weiss, D. Meier, W. Zhao, S. Tömekce, M. G. Cuxart, B. P. Klein, D. A. Duncan, T.-L. Lee, A. C. Papageorgiou, M. Muntwiler, A. P. Seitsonen, W. Auwärter, P. Feulner, J. V. Barth, and F. Allegretti, Phys. Rev. Materials **8**, 104001 (2024).