Band structure of chiral magnet Yb(Ni,*M*)$_3$Al$_9$ (*M*=Pd,Pt) observed by ARPES

Y. Murakami[a], Y. Tanimoto[b], Y. Nakashima[b], K. Kimura[b], H. Sato[c], K. Tanaka[d], K. Yamagami[e], S. Nakamura[f], S. Ohara[f]

[a]*Faculty of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*
[b]*Graduate School of Advanced Science and Engineering, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*
[c]*Hiroshima Research Institute for Synchrotron Radiation Science, Hiroshima University, Higashi-Hiroshima 739-0046, Japan*
[d]*UVSOR synchrotron Facility, Institute for Molecular Science*
[e]*Japan Synchrotron Radiation Research Institute*
[f]*Japan Graduate School of Engineering, Nagoya Institute of Technology*

Keywords: chiral magnetic crystal, helical magnetism, angle resolved photoemission spectroscopy

Trigonal $YbNi_3Al_9$ with a chiral crystal structure is of interest as the first chiral magnetic metal discovered among 4*f* electron systems [1]. The localized Yb 4*f* moments are magnetically ordered below T=3.4 K, ferromagnetically aligned within the *c*-plane, and exhibit either left-handed or right-handed helical magnetic structures with a propagation vector $\boldsymbol{q}$=(0, 0, 0.8) along the c-axis [2]. Owing to its chiral crystal structure, spin splitting in the conduction-electron band structure is expected, which is considered to play an essential role in the emergence of chiral magnetism. Furthermore, partial substitution of Ni with the heavier isovalent elements Pd and Pt is anticipated to enhance the spin splitting due to the increased spin-orbit interaction. In this study, we performed vacuum ultraviolet angle-resolved photoemission spectroscopy (VUV-ARPES) and soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) on $YbNi_3Al_9$ and its 5% substituted compounds, $Yb(Ni_{0.95}Pd_{0.05})Al_9$ and $Yb(Ni_{0.95}Pt_{0.05})Al_9$, to investigate the electronic structure near the Fermi level (E_F). The VUV-ARPES and SX-ARPES measurements were carried out at BL7U of UVSOR-III and BL25SU of SPring-8, respectively. Single crystals used for the measurements were synthesized by the flux-method [3]. First-principles band-structure calculations were carried out using the WIEN2k code [4], and the results were compared with the experimental data.

At $h\nu$ = 24 eV and T = 10 K, VUV-ARPES spectra of $YbNi_3Al_9$ measured with *s*-polarized light along the $\bar{\Gamma}$-$\bar{M}$ direction reveal two hole-like bands crossing E_F and an upward-convex parabolic band centered at the $\bar{\Gamma}$ point. Similar band dispersions were observed for $Yb(Ni_{0.95}Pd_{0.05})Al_9$ and $Yb(Ni_{0.95}Pt_{0.05})Al_9$. Within the experimental accuracy, no clear enhancement of the spin-splitting width was detected upon Pd or Pt substitution, which is likely due to the relatively small substitution level (5%). The Fermi surface of $YbNi_3Al_9$ measured at $h\nu$ = 510 eV and T = 70 K using circularly polarized light consists of at least two sixfold-symmetric hole sheets centered at the $\bar{\Gamma}$ point and electron sheets around the $\bar{K}$ points. The overall band dispersions and Fermi-surface topology are qualitatively reproduced by the band calculations. A comparison with calculations for the hypothetical compound $YbPt_3Al_9$ indicates that the spin splitting is significantly enhanced in the outermost hole band around the $\bar{\Gamma}$ point, suggesting that stronger spin-orbit coupling can substantially modify the conduction-band spin splitting.

REFERENCES

1. S. Ohara, S. Fukuta, K. Ohta, H. Kono, T. Yamashita, Y. Matsumoto and J. Yamaura, JPS Conf. Proc. **3**, 017016 (2014).
2. T. Matsumura, Y. Kita, K. Kubo, Y. Yoshikawa, S. Michimura, T. Inami, Y. Kousaka, K. Inoue and S. Ohara, J. Phys. Soc. Jpn. **86**, 124702 (2017).
3. T. Yamashita, R. Miyazaki, Y. Aoki and S. Ohara, J. Phys. Soc. Jpn. **81**, 034705 (2012).
4. P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G. K. H. Madsen and L. D. Marks, J. Chem. Phys. **152**, 074101 (2020).