

東北大学 電気通信研究所  
**研究室外部評価 参考資料**  
(2013 年度-2018 年度)

**Research Laboratory Reference Data  
for External Review**

April 2013 – March 2019  
(FY. 2013–2018)

**Research Institute of Electrical Communication  
Tohoku University**

物性機能設計研究室

Materials Functionality Design

## 1. 研究成果 / Research Achievements

### (1) 査読付学術論文 / Refereed journal papers

(FY2013)

[1] Y. Miura, M. Tsujikawa and M. Shirai, "A first-principles study on magnetocrystalline anisotropy at interfaces of Fe with non-magnetic metals," J. Appl. Phys., Vol. 113, No. 23, Article No. 233908, pp. 1-6, 2013.

[2] K. Abe and N.W. Ashcroft, "Quantum disproportionation: The high hydrides at elevated pressures," Phys. Rev. B, Vol. 88, No. 17, Article no. 174110, pp. 1-5, 2013.

[3] Y. Miura and M. Shirai, "Theoretical study on tunneling magnetoresistance of manetic tunnel junctions with  $D0_{22}$ - $Mn_3Z$  ( $Z = Ga, Ge$ )," IEEE Trans. Magn., Vol. 50, No. 1, Article No. 1400504, pp. 1-4, 2014.

[4] G.-f. Li, Y. Honda, H.-x. Liu, K. Matsuda, M. Arita, T. Uemura, M. Yamamoto, Y. Miura, M. Shirai, T. Saito, F. Shi, and P. M. Voyles, "Effect of non-stoichiometry on the half-metallic character of  $Co_2MnSi$  investigated through saturation magnetization and tunneling spin polarization," Phys. Rev. B, Vol. 89, No. 1, Article No. 014428, pp. 1-14, 2014.

(FY2014)

[1] S. Ueda, M. Mizuguchi, T. Kojima, S. Ishimaru, M. Tsujikawa, M. Shirai, and K. Takanashi, "Detection of spin-resolved electronic structures from a buried ferromagnetic layer utilizing forward Mott scattering," Appl. Phys. Lett., Vol. 104, No. 13, Article No. 132402, pp.1-5, 2014.

[2] H. Nishihara, K. Suzuki, R. Y. Umetsu, T. Kanomata, T. Kaneko, M. Y. Zhou, M. Tsujikawa, M. Shirai, T. Sakon, T. Wada, K. Terashima, and S. Imada, "Magnetic properties of  $Ni_2N$ ," Physica B, Vol. 449, pp.85-89, 2014.

[3] S. Kanai, M. Tsujikawa, Y. Miura, M. Shirai, F. Matsukura, and H. Ohno, "Magnetic anisotropy in Ta/CoFeB/MgO investigated by x-ray magnetic circular dichroism and first-principles calculation," Appl. Phys. Lett., Vol. 105, No. 22, Article No. 222409, pp.1-4, 2014.

(FY2015)

[1] V. R. Singh, V. K. Verma, K. Ishigami, G. Shibata, A. Fujimori, T. Koide, Y. Miura, M. Shirai, T. Ishikawa, G.-f. Li, and M. Yamamoto, "Electronic and magnetic properties of off-stoichiometric  $Co_2Mn_\beta Si/MgO$  interfaces studied by x-ray magnetic circular dichroism," J. Appl. Phys., Vol. 117, No. 20, Article No. 203901, pp. 1-6, 2015.

[2] S. Zhu, M. Ye, K. Shirai, M. Taniguchi, S. Ueda, Y. Miura, M. Shirai, R. Y. Umetsu, R. Kainuma, T. Kanomata, and A. Kimura, "Drastic change in density of states upon martensitic phase transition for metamagnetic shape memory alloy  $Ni_2Mn_{1+x}In_{1-x}$ ," J. Phys.: Condens. Matter, Vol. 27, No. 36, Article No. 362201, pp. 1-6, 2015.

[3] K. Abe and N. W. Ashcroft, "Stabilization and highly metallic properties of heavy group-V hydrides at high pressures," Phys. Rev. B, Vol. 92, No. 22, Article No. 224109, pp. 1-5, 2015.

(FY2016)

[1] K. Moges, Y. Honda, H.-x. Liu, T. Uemura, M. Yamamoto, Y. Miura, and M. Shirai, "Enhanced half-metallicity of off-stoichiometric quaternary Heusler alloy  $Co_2(Mn,Fe)Si$  investigated through saturation magnetization and tunneling magnetoresistance," Phys. Rev. B, Vol. 93, No. 13, Article no. 134403, pp. 1-15, 2016.

[2] S. Ueda, M. Mizuguchi, Y. Miura J. G. Kang, M. Shirai, and K. Takanashi, "Electronic structure and magnetic anisotropy of  $L1_0$ -FePt thin film studied by hard x-ray photoemission spectroscopy and first-principles calculations," Appl. Phys. Lett., Vol. 109, No. 4, Article no. 042404, pp. 1-5, 2016.

[3] B. Hu, K. Moges, Y. Honda, H.-x. Liu, T. Uemura, M. Yamamoto, J. Inoue, and M. Shirai, "Temperature dependence of spin-dependent tunneling conductance of magnetic tunnel junctions with half-metallic  $Co_2MnSi$  electrodes," Phys. Rev. B, Vol. 94, No. 9, Article no.

094428, pp. 1-15, 2016.

[4] T. Kubota, Y. Ina, M. Tsujikawa, S. Morikawa, H. Narisawa, Z. Wen, M. Shirai, and K. Takanashi, "Current perpendicular-to-plane giant magnetoresistance devices using half-metallic  $\text{Co}_2\text{Fe}_{0.4}\text{Mn}_{0.6}\text{Si}$  electrodes and a Ag-Mg spacer layer," J. Phys. D: Appl. Phys., Vol. 50, No. 1, Article no. 014004, pp. 1-8, 2017.

(FY2017)

[1] J. Okabayashi, T. Koyama, M. Suzuki, M. Tsujikawa, M. Shirai and D. Chiba, "Induced perpendicular magnetization in a Cu layer inserted between Co and Pt layers revealed by x-ray magnetic circular dichroism," Sci. Rep., Vol. 7, Article no. 46132, pp. 1-9, 2017.

[2] S. Miwa, M. Suzuki, M. Tsujikawa, K. Matsuda, T. Nozaki, K. Tanaka, T. Tsukahara, K. Nawaoka, M. Goto, Y. Kotani, T. Ohkubo, F. Bonell, E. Tamura, K. Hono, T. Nakamura, M. Shirai, S. Yuasa and Y. Suzuki, "Voltage control of platinum orbit: A contribution to interfacial magnetism," Nature Commun., Vol. 8, Article no. 15848, pp. 1-9, 2017.

[3] T. Seki, J. Shimada, S. Iihama, M. Tsujikawa, T. Koganezawa, A. Shioda, T. Tashiro, W. Zhou, S. Mizukami, M. Shirai and K. Takanashi, "Magnetic anisotropy and damping for monolayer-controlled Co/Ni epitaxial multilayer," J. Phys. Soc. Jpn., Vol. 86, No. 7, Article no. 074710, pp. 1-10, 2017.

[4] K. Abe, "Hydrogen-rich scandium compounds at high pressures," Phys. Rev. B, Vol. 96, No. 14, Article no. 144108, pp. 1-7, 2017.

[5] T. Nozaki, A. Koziol-Rachwal, M. Tsujikawa, Y. Shiota, X. Xu, T. Ohkubo, T. Tsukahara, S. Miwa, M. Suzuki, S. Tamaru, H. Kubota, A. Fukushima, K. Hono, M. Shirai, Y. Suzuki and S. Yuasa, "Highly efficient voltage control of spin and enhanced interfacial perpendicular magnetic anisotropy in iridium-doped Fe/MgO magnetic tunnel junctions," NPG Asia Mater., Vol. 9, Article no. e451, pp. 1-10, 2017.

[6] S. Souma, K. Honma, T. Sato, M. Tsujikawa, M. Shirai and T. Takahashi, "Emergence of undulating surface band upon oxygen adsorption of Fe thin film on W(110)," Appl. Phys. Lett., Vol. 111, No. 24, Article no. 241603, pp. 1-4, 2017.

[7] T. Kawabe, K. Yoshikawa, M. Tsujikawa, T. Tsukahara, K. Nawaoka, Y. Kotani, K. Toyoki, M. Goto, M. Suzuki, T. Nakamura, M. Shirai, Y. Suzuki and S. Miwa, "Electric-field-induced magnetic moments and magnetocrystalline anisotropy in cobalt ultrathin films," Phys. Rev. B, Vol. 96, Article no. 220412(R), pp. 1-6, 2017.

[8] L. Bainsla, K. Z. Suzuki, M. Tsujikawa, H. Tsushiura, M. Shirai and S. Mizukami, "Magnetic tunnel junctions with an equiatomic quaternary CoFeMnSi Heusler alloy electrode," Appl. Phys. Lett., Vol. 112, No. 5, Article no. 052403, pp. 1-5, 2018.

[9] I. Shigeta, Y. Fujimoto, R. Ooka, Y. Nishisako, M. Tsujikawa, R. Y. Umetsu, A. Nomura, K. Yubuta, Y. Miura, T. Kanomata, M. Shirai, J. Gouchi, Y. Uwatoko and M. Hiroi, "Pressure effect on magnetic properties of half-metallic Heusler alloy  $\text{Co}_2\text{TiSn}$ ," Phys. Rev. B, Vol. 97, No. 10, Article no. 104414, pp.1-8, 2018.

(FY2018)

[1] L. Bainsla, R. Yilgin, M. Tsujikawa, K. Z. Suzuki, M. Shirai and S. Mizukami, "Low magnetic damping for equiatomic CoFeMnSi Heusler alloy," J. Phys. D: Appl. Phys., Vol. 51, Article no. 495001, pp. 1-7, 2018.

[2] Y. Goto, M. Araki, N. Takahashi, T. Yanase, T. Shimada, M. Tsujikawa, M. Shirai, A. Kamimaki, S. Iihama, S. Mizukami and T. Nagahama, "Synthesis of metastable B2-type Fe-Sn alloy epitaxial films and study of their magnetic properties," Jpn. J. Appl. Phys., Vol. 57, Article no. 120302, pp. 1-5, 2018.

[3] K Abe, "High-pressure properties of dense metallic zirconium hydrides studied by *ab initio* calculations," Phys. Rev. B, Vol. 98, Article No. 134103, pp. 1-7, 2018.

[4] R. Y. Umetsu, M. Tsujikawa, K. Saito, K. Ono, T. Ishigaki, R. Kainuma and M. Shirai, "Atomic ordering, magnetic properties, and electronic structure of  $\text{Mn}_2\text{CoGa}$  Heusler alloy," J. Phys.: Condens. Matter, Vol. 31, Article no. 065801, pp. 1-10, 2019.

[5] Y. Jibiki, M. Goto, M. Tsujikawa, P. Risius, S. Hasebe, X. Xu, K. Nawaoka, T. Ohkubo,

K. Hono, M. Shirai, S. Miwa and Y. Suzuki, "Interface resonance in Fe/Pt/MgO multilayer structure with large voltage controlled magnetic anisotropy change," Appl. Phys. Lett., Vol. 114, Article no. 082405, pp. 1-5, 2019.

(2) 原著論文と同等に扱う査読付国際会議発表論文

Full papers in refereed conference proceedings equivalent to journal papers

該当なし N/A

(3) 査読付国際会議 / Presentations in refereed conferences

(FY2013)

[1] M. Tsujikawa, D. Mori, Y. Miura, and M. Shirai, "Perpendicular magnetic anisotropy and its electrical modulation of MgO/Co<sub>2</sub>FeAl interface: A first-principles study," Yamada Conference LXVII - 8th International Symposium on Metallic Multilayers, Kyoto, Japan, (19-24 May, 2013).

[2] M. Mizuguchi, T. Kojima, S. Ozaki, Y. Miura, M. Shirai, and K. Takanashi, "Perpendicular magnetic anisotropy in artificially fabricated L1<sub>0</sub>-FeNi thin films," Yamada Conference LXVII - 8th International Symposium on Metallic Multilayers, Kyoto, Japan, (19-24 May, 2013).

[3] S. Ozaki, M. Tsujikawa, Y. Miura, K. Abe, and M. Shirai, "A first-principles study on magnetic anisotropy of Fe/Ni multilayers." Yamada Conference LXVII - 8th International Symposium on Metallic Multilayers, Kyoto, Japan, (19-24 May, 2013).

[4] S. Ueda, M. Mizuguchi, J. G. Kang, Y. Miura, M. Shirai, and K. Takanashi, "Electronic structure of L1<sub>0</sub> ordered FePt thin film." 5th International Conference on Hard X-ray Photoelectron Spectroscopy, Uppsala, Sweden, (17-20 June, 2013).

[5] Y. Miura and M. Shirai, "Theoretical study on tunneling magnetoresistance of manetic tunnel junctions with D0<sub>22</sub>-Mn<sub>3</sub>Z (Z = Ga, Ge)," 3rd International Symposium on Advanced Magnetic Materials and Applications, Taichung, Taiwan, (21-25 July, 2013).

[6] M. Tsujikawa, Y. Miura, and M. Shirai, "The influence of Co and B atoms on the perpendicular magnetic anisotropy of MgO/CoFeB film," 3rd International Symposium on Advanced Magnetic Materials and Applications, Taichung, Taiwan, (21-25 July, 2013).

[7] S. Ueda, M. Mizuguchi, J. G. Kang, Y. Miura, M. Shirai, and K. Takanashi, "Electronic and magnetic states of L1<sub>0</sub> ordered FePt thin film," International Conference on Nanoscale Magnetism 2013, Istanbul, Turkey, (2-6 September, 2013).

[8] S. Ueda, M. Mizuguchi, T. Kojima, S. Ishimaru, M. Tsujikawa, M. Shirai, K. Takanashi, and O. Sakata, "New approach to spin-resolved photoemission using hard x-rays: Electronic and magnetic states of an FeNi film buried under a Au thin film," 58th Annual Conference on Magnetism and Magnetic Materials, Denver, Colorado, USA, (4-8 November, 2013).

(FY2014)

[1] M. Tsujikawa, Y. Miura, and M. Shirai, "Perpendicular magnetic anisotropy in MgO/Co-based Heusler alloy junctions: A first-principles study," 15th IUMRS International Conference in Asia, Fukuoka, Japan, (24-30 August, 2014).

[2] K. Moges, Y. Honda, T. Uemura, M. Yamamoto, Y. Miura, and M. Shirai, "Effect of nonstoichiometry on the half-metallicity of Co<sub>2</sub>(Mn,Fe)Si thin films investigated through saturation magnetization," 59th Annual Conference on Magnetism and Magnetic Materials, Honolulu, Hawaii, USA, (3-7 November, 2014).

[3] S. Ueda, M. Mizuguchi, T. Kojima, S. Ishimaru, M. Tsujikawa, M. Shirai, and K. Takanashi, "Detection of spin-resolved electronic structures from a buried ferromagnetic layer utilizing forward Mott scattering," 59th Annual Conference on Magnetism and Magnetic Materials, Honolulu, Hawaii, USA, (3-7 November, 2014).

[4] M. Mizuguchi, S. Ueda, Y. Miura, T. Kojima, M. Shirai, and K. Takanashi, "Electronic structures of L1<sub>0</sub>-ordered FeNi thin films studied by photoelectron spectroscopy," 59th Annual Conference on Magnetism and Magnetic Materials, Honolulu, Hawaii, USA, (3-7

November, 2014).

(FY2015)

[1] M. Tsujikawa and M. Shirai, "Electronic structure and magnetic properties of  $Mn_3Ga$  doped with Ti, V, and Cr: A first-principles study," 2016 Joint Magnetism and Magnetic Materials/International Magnetism Conference, San Diego, California, USA, (11-15 January, 2016).

(FY2016)

[1] M. Tsujikawa, T. Ito, and M. Shirai, "First-principles study on the magnetic anisotropy and magnetic damping in hexagonal Fe/Co, Co/Ni, Fe/Ni multilayers," 9th International Symposium on Metallic Multilayers, Uppsala, Sweden, (19-23 June, 2016).

[2] M. Shirai, A. Onodeta, M. Tsujikawa, and Y. Miura, "First-principles calculation of electronic structure in NiMnSb/MgO and CoMnSb/MgO junctions," 4th International Conference of Asian Union of Magnetism Societies, Tainan, Taiwan, (1-5 August, 2016).

[3] M. Tsujikawa, S. Kano, and M. Shirai, "First-principles study on the magnetostructural phase transitions of Co-based Heusler alloys," 5th International Conference on Ferromagnetic Shape Memory Alloys, Sendai, Japan, (5-9 September, 2016).

[4] Y. Miura, M. Tsujikawa, and M. Shirai, "Electric field dependence of magnetic damping of Fe-layer: A first-principles study," 61st Annual Conference on Magnetism and Magnetic Materials, New Orleans, Louisiana, USA, (31 October - 4 November, 2016).

(FY2017)

[1] M. Tsujikawa and M. Shirai, "Enhancement of magnetization in Mn-Ga alloys doped with typical elements: A first-principles study," IEEE International Magnetism Conference 2017, Dublin, Ireland, (24-28 April, 2017).

[2] M. Tsujikawa and M. Shirai, "Huge voltage-induced magnetic anisotropy change of 5d transition-metals on Fe(001) and Co(0001)," IEEE International Magnetism Conference 2017, Dublin, Ireland, (24-28 April, 2017).

[3] M. Tsujikawa and M. Shirai, "Huge electric-field-induced magnetic anisotropy of the 5d transition-metal monolayers on Fe(001) and Co(0001)," 28th Magnetic Recording Conference, Tsukuba, Japan, (2-4 August, 2017).

[4] K. Sumida, M. Tsujikawa, X. Xu, J. Chen, S. Zhu, T. Yoshikawa, S. Higaki, S. Ueda, Y. Takeda, Y. Saitoh, M. Shirai, R. Kainuma, and A. Kimura, "Unveiling reentrant martensitic phase transition mechanism in  $Co_2Cr(Ga,Si)$  Heusler alloys," Yamada Science Foundation Junjiro Kanamori Memorial International Symposium – New Horizon of Magnetism –, Tokyo, Japan, (27-29 September, 2017).

[5] S. Kumata, M. Tsujikawa, and M. Shirai, "Giant modulation of magnetization induced by electric polarization reversal at  $Fe_4N/BaTiO_3$  interface," 62nd Annual Conference on Magnetism and Magnetic Materials, Pittsburgh, Pennsylvania, USA, (6-10 November, 2017).

[6] Y. Mitsuhashi, M. Tsujikawa, and M. Shirai, "Theoretical design of Mn-based ordered alloys with high magnetization by lattice expansion," 62nd Annual Conference on Magnetism and Magnetic Materials, Pittsburgh, Pennsylvania, USA, (6-10 November, 2017).

[7] M. Suzuki, M. Tsujikawa, T. Nozaki, T. Tsukahara, T. Kawabe, K. Shimose, T. Furuta, R. Miyakaze, K. Yoshikawa, K. Nawaoka, M. Goto, Y. Kotani, K. Toyoki, T. Nakamura, T. Ohkubo, K. Hono, M. Shirai, S. Yuasa, Y. Suzuki, and S. Miwa, "X-ray magnetic circular dichroism spectroscopy to study the microscopic origin of voltage-induced magnetic anisotropy in ferromagnetic metal/MgO interfaces," 4th International Symposium on Advanced Magnetic Materials and Applications, Phu Quoc Island, Vietnam, (December 10-13 1, 2017).

[8] S. Miwa, M. Suzuki, M. Tsujikawa, K. Matsuda, T. Nozaki, K. Tanaka, M. Goto, Y. Kotani, T. Ohkubo, F. Bonell, E. Tamura, K. Hono, T. Nakamura, M. Shirai, and Y. Suzuki,

“Microscopic origin of voltage-controlled magnetic anisotropy in FePt/MgO epitaxial multilayer,” APS March Meeting 2018, Los Angeles, California, USA, (March 5-9, 2018).

[9] T. Kawabe, K. Yoshikawa, M. Tsujikawa, T. Tsukahara, K. Nawaoka, Y. Kotani, K. Toyoki, M. Goto, M. Suzuki, T. Nakamura, M. Shirai, Y. Suzuki, and S. Miwa, “Electric-field-induced changes in magnetic moments and magnetic anisotropy in Co/MgO multilayer,” APS March Meeting 2018, Los Angeles, California, USA, (March 5-9, 2018).

(FY2018)

[1] L. Bainsla, K. Z. Suzuki, M. Tsujikawa, H. Tsuchiura, M. Shirai, and S. Mizukami, “Tunneling magnetoresistance effect with an equiatomic CoFeMnSi Heusler alloy electrode,” 21st International Conference on Magnetism (ICM 2018), San Francisco, California, USA, (16-20 July, 2018).

[2] S. Ueda, M. Mizuguchi, M. Tsujikawa, and M. Shirai, “Electronic structures and magnetic properties of Fe/MgO interfaces studied by hard x-ray photoelectron spectroscopy,” 21st International Conference on Magnetism (ICM 2018), San Francisco, California, USA, (16-20 July, 2018).

[3] T. Nagahama, Y. Goto, M. Araki, T. Yanase, T. Shimada, M. Tsujikawa, and M. Shirai, “Fabrication of metastable B2 Fe<sub>1-x</sub>Sn<sub>x</sub> films by epitaxial growth on MgO(001),” 23rd International Colloquium on Magnetic Films and Surfaces (ICMFS 2018), Santa Cruz, California, USA, (22-27 July, 2018).

[4] L. Bainsla, K. Z. Suzuki, M. Tsujikawa, H. Tsuchiura, M. Shirai, and S. Mizukami, “Magnetic tunnel junctions with an equiatomic CoFeMnSi electrode,” International Conference on Solid State Devices and Materials (SSDM 2018), Tokyo, Japan, (9-13 September, 2018).

[5] M. Tsujikawa and M. Shirai, “Enhancement of voltage-controlled magnetic anisotropy by Ir doping in Co-based Heusler alloys,” 2019 Joint Magnetism and Magnetic Materials/International Magnetism (MMM-Intermag) Conference, Washington, DC, USA, (14-18 January, 2019).

[6] T. Kanemura, T. Roy, M. Tsujikawa, and M. Shirai, “Theoretical prediction of new quaternary Heusler alloys having high Curie temperatures and high spin polarizations with the aid of machine learning,” 2019 Joint Magnetism and Magnetic Materials/International Magnetism (MMM-Intermag) Conference, Washington, DC, USA, (14-18 January, 2019).

[7] Y. Goto, M. Araki, N. Takahashi, T. Yanase, T. Shimada, M. Tsujikawa, M. Shirai, A. Kamimaki, S. Iihama, S. Mizukami, and T. Nagahama, “Fabrication of metastable B2-type Fe<sub>1-x</sub>Sn<sub>x</sub> epitaxial films on MgO(001) substrates,” 2019 Joint Magnetism and Magnetic Materials/International Magnetism (MMM-Intermag) Conference, Washington, DC, USA, (14-18 January, 2019).

[8] L. Bainsla, R. Yilgin, M. Tsujikawa, K. Z. Suzuki, M. Shirai, and S. Mizukami, “Low Gilbert damping for epitaxial thin films of the equiatomic CoFeMnSi Heusler alloy,” 2019 Joint Magnetism and Magnetic Materials/International Magnetism (MMM-Intermag) Conference, Washington, DC, USA, (14-18 January, 2019).

[9] T. Tsuchiya, T. Roy, K. Elphick, L. Bainsla, M. Tsujikawa, M. Shirai, A. Hirohata, and S. Mizukami, “Magnetization dynamics for the equiatomic Heusler CoFeCrAl alloy epitaxial films and spin-dependent transport in their magnetic tunnel junctions,” 2019 Joint Magnetism and Magnetic Materials/International Magnetism (MMM-Intermag) Conference, Washington, DC, USA, (14-18 January, 2019).

#### (4) 査読なし国際会議・シンポジウム等 / Presentations in conferences

(FY2013)

[1] Y. Miura and M. Shirai, “Theoretical studies on spin-dependent transport phenomena in heterostructures based on half-metallic Heusler alloys,” Annual Meeting of Strategic Japanese-German Joint Research Program “ASPIMATT”: Advanced Spintronic Materials and Transport Phenomena, Dresden, Germany, (4-5 July, 2013).

[2] M.-Y. Zhou, Y. Miura, K. Abe, and M. Shirai, “Theoretical study on spin-dependent transport properties in magnetic tunnel junctions with Fe<sub>4</sub>N electrodes,” Annual Meeting of

Strategic Japanese-German Joint Research Program “ASPIMATT”: Advanced Spintronic Materials and Transport Phenomena, Dresden, Germany, (4-5 July, 2013).

[3] T. Ito, M. Tsujikawa, Y. Miura, K. Abe, and M. Shirai, “A first-principles study on magnetic anisotropy of L1<sub>1</sub>-ordered CoNi,” Annual Meeting of Strategic Japanese-German Joint Research Program “ASPIMATT”: Advanced Spintronic Materials and Transport Phenomena, Dresden, Germany, (4-5 July, 2013).

[4] S. Kano, M. Tsujikawa, Y. Miura, K. Abe, and M. Shirai, “First-principles study on the magnetocrystalline anisotropy of Co-based Heusler alloys,” Annual Meeting of Strategic Japanese-German Joint Research Program “ASPIMATT”: Advanced Spintronic Materials and Transport Phenomena, Dresden, Germany, (4-5 July, 2013).

[5] A. Onodera, S. Tanibayashi, and M. Shirai, “Computational study on transport properties of single molecule junction with magnetic electrodes,” Annual Meeting of Strategic Japanese-German Joint Research Program “ASPIMATT”: Advanced Spintronic Materials and Transport Phenomena, Dresden, Germany, (4-5 July, 2013).

(FY2014)

[1] Y. Miura and M. Shirai, “Theoretical studies on spin-dependent transport phenomena in heterostructures based on half-metallic Heusler alloys,” Annual Meeting of Strategic Japanese-German Joint Research Program “ASPIMATT”: Advanced Spintronic Materials and Transport Phenomena, Sendai, Japan, (30-31 October, 2014).

(FY2015)

[1] M. Tsujikawa and M. Shirai, “The effect of light-element doping on magnetic anisotropy in L1<sub>0</sub>-FeNi: A first-principles study,” ESICMM-G8 Symposium on Next Generation Permanent Magnets, Tsukuba, Japan, (18-19 June, 2015).

(FY2017)

[1] M. Tsujikawa and M. Shirai, “Magnetic anisotropy and magnetic damping in hexagonal Co/Ni multilayers,” York-Tohoku-Kaiserslautern Research Symposium on “New-Concept Spintronics Devices”, York, UK, (21-23 June, 2017).

[2] T. Kanemura, M. Tsujikawa, and M. Shirai, “*Ab initio* calculation of electric-field effect on magnetic anisotropy at Fe/MgO interfaces: The role of lattice distortion,” York-Tohoku-Kaiserslautern Research Symposium on “New-Concept Spintronics Devices”, York, UK, (21-23 June, 2017).

[3] Y. Saito, T. Kanemura, M. Tsujikawa, and M. Shirai, “Electric-field control of magnetic anisotropy in Cu/Co/Pd layers: *Ab initio* calculation,” York-Tohoku-Kaiserslautern Research Symposium on “New-Concept Spintronics Devices”, York, UK, (21-23 June, 2017).

[4] S. Miwa, M. Suzuki, M. Tsujikawa, T. Nozaki, T. Tsukahara, T. Kawabe, K. Yoshikawa, K. Nawaoka, M. Goto, Y. Kotani, K. Toyoki, T. Nakamura, T. Ohkubo, K. Hono, M. Shirai, S. Yuasa, and Y. Suzuki, “Microscopic origin of voltage-controlled magnetic anisotropy in ferromagnetic thin-film metals,” 3rd ImPACT International Symposium on Spintronic Memory, Circuit and Storage, Sendai, Japan, (September 23-25, 2017).

[5] M. Tsujikawa and M. Shirai, “Huge voltage-induced magnetic anisotropy change in the 5d transition-metal monolayer on the Fe and Co surface,” 3rd ImPACT International Symposium on Spintronic Memory, Circuit and Storage, Sendai, Japan, (September 23-25, 2017).

[6] S. Kumata, M. Tsujikawa, and M. Shirai, “Giant interfacial magnetoelectric effect and transport properties in Fe<sub>4</sub>N/BaTiO<sub>3</sub>/Fe magnetic tunnel junctions,” 15th RIEC International Workshop on Spintronics and 6th JSPS Core-to-Core Workshop on “New-Concept Spintronics Devices”, Sendai, Japan, (15-16 December, 2017).

[7] M. Tsujikawa and M. Shirai, “First-principles study on magnetic anisotropy and damping of Co/Ni multilayers,” Kick-off Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan, (19-20 February, 2018).

[8] M. Tsujikawa and M. Shirai, “Origin of voltage-controlled magnetic anisotropy in FeCo

and FePt thin films,” Kick-off Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan, (19-20 February, 2018).

[9] S. Kumata, M. Tsujikawa, and M. Shirai, “Interfacial magnetoelectric coupling and transport properties in  $\text{Fe}_4\text{N}/\text{BaTiO}_3/\text{Fe}$  magnetic tunnel junctions,” Kick-off Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan, (19-20 February, 2018).

[10] Y. Mitsuhashi, M. Tsujikawa, and M. Shirai, “Theoretical design of  $\text{DO}_{22}$ -type ordered alloys with high magnetization by lattice expansion,” Kick-off Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan, (19-20 February, 2018).

[11] T. Kanemura, M. Tsujikawa, and M. Shirai, “Prediction of the magnetization in transition-metal binary alloys by means of machine learning,” Kick-off Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan, (19-20 February, 2018).

(FY2018)

[1] R. Okado, M. Tsujikawa, and M. Shirai, “Theoretical study on interfacial magnetic anisotropy at ZnO/Co interfaces,” 7th Workshop Core-to-Core Project Tohoku-York-Kaiserslautern “New-Concept Spintronics Devices”, Kaiserslautern, Germany, (28-30 May, 2018).

[2] M. Tsujikawa, and M. Shirai, “Enhancement of the voltage-controlled magnetic anisotropy by Ir doping at the MgO/Fe interface,” 7th Workshop Core-to-Core Project Tohoku-York-Kaiserslautern “New-Concept Spintronics Devices”, Kaiserslautern, Germany, (28-30 May, 2018).

[3] T. Tsuchiya, T. Roy, K. Elphick, L. Bainsla, M. Tsujikawa, M. Shirai, A. Hirohata, and S. Mizukami, “Annealing temperature dependence of tunnel magnetoresistance effects of CoFeCrAl Heusler alloy,” 2nd Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan, (16-18 February, 2019).

[4] M. Tsujikawa and M. Shirai, “Enhancement of voltage-controlled magnetic anisotropy by lattice distortion in FeCo films,” 2nd Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan, (16-18 February, 2019).

(5) 総説・解説 / Review articles

(FY2018)

[1] 阿部和多加, “水素と水素化合物の金属相探索,” 高圧力の科学と技術, Vol. 28, pp. 281-290, (2018);

[K. Abe, “Search for Metallic Phases of Hydrogen and Hydrides,” Rev. High Pressure Sci. Technol., Vol. 28, pp. 281-290, (2018)].

[2] S. Miwa, M. Suzuki, M. Tsujikawa, T. Nozaki, T. Nakamura, M. Shirai, S. Yuasa and Y. Suzuki, “Perpendicular magnetic anisotropy and its electric-field-induced change at metal-dielectric interfaces,” J. Phys. D: Appl. Phys., Vol. 52, Article no. 063001, pp. 1-22, (2019).

(6) 査読付国内会議 / Presentations in refereed domestic conferences

(FY2013)

[1] 本田佑輔, 李桂芳, 劉宏喜, 有田正志, 松田健一, 植村哲也, 山本眞史, 齊藤敏明, 三浦良雄, 白井正文, “ $\text{Co}_2\text{MnSi}$  薄膜の飽和磁化およびトンネルスピン偏極率に対する非化学量論的組成の影響,” (3p C-7), 第 37 回 日本磁気学会 学術講演会, 北海道大学, (2013 年 9 月 3 日);

[Y. Honda, G.-f. Li, H.-x. Liu, M. Arita, K. Matsuda, T. Uemura, M. Yamamoto, T. Saito, Y. Miura, and M. Shirai, “Effect of nonstoichiometry on the half-metallicity of  $\text{Co}_2\text{MnSi}$  thin films with various Mn compositions,” (3p C-7), 37th Annual Conference on Magnetism in Japan, Hokkaido Univ., (3 September, 2013)].

[2] 辻川雅人, 森大樹, 三浦良雄, 白井正文, “MgO/ $\text{Co}_2\text{FeAl}$  界面における垂直磁気異方性



- の電界変調,” (18a C15-1), 2013 年 第 74 回 応用物理学会 秋季学術講演会, 同志社大学, (2013 年 9 月 18 日);
- [M. Tsujikawa, D. Mori, Y. Miura, and M. Shirai, “Electric-field modulation of perpendicular magnetic anisotropy at MgO/Co<sub>2</sub>FeAl interface,” (18a C15-1), 74th JSAP Autumn Meeting 2013, Doshisha Univ., (18 September, 2013)].
- [3] 谷林慧, 三浦良雄, 白井正文, “Mn<sub>3-δ</sub>X<sub>δ</sub>Ga (X = Fe, Co, Ni) の電子状態に関する第一原理計算,” (18a C15-2), 2013 年 第 74 回 応用物理学会 秋季学術講演会, 同志社大学, (2013 年 9 月 18 日);
- [S. Tanibayashi, Y. Miura, and M. Shirai, “A first-principles study on the electronic structure of Mn<sub>3-δ</sub>X<sub>δ</sub>Ga (X = Fe, Co, Ni),” (18a C15-2), 74th JSAP Autumn Meeting 2013, Doshisha Univ., (18 September, 2013)].
- [4] 尾崎翔, 三浦良雄, 辻川雅人, 阿部和多加, 白井正文, “FeNi 多層膜の結晶磁気異方性に関する第一原理計算,” (18a C15-8), 2013 年 第 74 回 応用物理学会 秋季学術講演会, 同志社大学, (2013 年 9 月 18 日);
- [S. Ozaki, Y. Miura, M. Tsujikawa, K. Abe, and M. Shirai, “A first-principles study on magneto-crystalline anisotropy of FeNi multilayers,” (18a C15-8), 74th JSAP Autumn Meeting 2013, Doshisha Univ., (18 September, 2013)].
- [5] 辻川雅人, 三浦良雄, 白井正文, “Co 基ホイスラー合金と MgO 界面における磁気異方性の第一原理計算,” (25a PS-13), 日本物理学会 2013 年秋季大会, 徳島大学, (2013 年 9 月 25 日);
- [M. Tsujikawa, Y. Miura, and M. Shirai, “Magnetic anisotropy of Co-based Heusler alloy and MgO interface: a first principles study,” (25a PS-13), Physical Society of Japan 2013 Autumn Meeting, Tokushima Univ., (25 September, 2013)].
- [6] 大槻匠, 小嗣真人, 大河内拓雄, 中村哲也, 小嶋隆幸, 荻原美沙子, 田代敬之, 水口将輝, 三浦良雄, 白井正文, 高梨弘毅, “X 線磁気円二色性による L<sub>10</sub> 型 FeNi 規則合金薄膜の磁気異方性評価,” (25a PS-40), 日本物理学会 2013 年秋季大会, 徳島大学, (2013 年 9 月 25 日);
- [T. Ohtsuki, T. Kojima, M. Kotsugi, T. Ohkochi, T. Nakamura, M. Ogiwara, T. Tashiro, M. Mizuguchi, Y. Miura, M. Shirai, and K. Takanashi, “Magnetic anisotropy of L<sub>10</sub>-type FeNi thin films studied by x-ray magnetic circular dichroism,” (25a PS-40), Physical Society of Japan 2013 Autumn Meeting, Tokushima Univ., (25 September, 2013)].
- [7] 三浦良雄, 尾崎翔, 辻川雅人, 白井正文, “第一原理計算による L<sub>10</sub> 型 FeNi の結晶磁気異方性に及ぼす元素添加の影響評価,” (25p PSB-13), 日本物理学会 2013 年秋季大会, 徳島大学, (2013 年 9 月 25 日);
- [Y. Miura, S. Ozaki, M. Tsujikawa, and M. Shirai, “A first-principles study on substitution effects on magnetocrystalline anisotropy of L<sub>10</sub>-FeNi,” (25p PSB-13), Physical Society of Japan 2013 Autumn Meeting, Tokushima Univ., (25 September, 2013)].
- [8] 阿部和多加, N. W. Ashcroft, “高圧における GeH<sub>3</sub> の安定性と超伝導,” (27a DF-9), 日本物理学会 2013 年秋季大会, 徳島大学, (2013 年 9 月 27 日);
- [K. Abe and N. W. Ashcroft, “Stability and superconductivity of GeH<sub>3</sub> at high pressures,” (27a DF-9), Physical Society of Japan 2013 Autumn Meeting, Tokushima Univ., (27 September, 2013)].
- [9] 寺嶋健成, 顧淳, 山田将太郎, 野中優, 東谷篤志, 関山明, 玉作賢治, 藤原秀紀, 山崎篤志, 恒川雅典, 菅滋正, 田中義人, 矢橋牧名, 石川哲也, 白井正文, 鹿又武, 今田真, “硬 X 線光電子分光を用いたホイスラー合金 Ni<sub>2</sub>MnGa の電子状態観測,” (28p DB-1), 日本物理学会 2013 年秋季大会, 徳島大学, (2013 年 9 月 28 日);
- [K. Terashima, *et al.*, “Observation of electronic states in a Heusler alloy Ni<sub>2</sub>MnGa using x-ray photoelectron spectroscopy,” (28p DB-1), Physical Society of Japan 2013 Autumn Meeting, Tokushima Univ., (28 September, 2013)].
- [10] 上田茂典, 水口将輝, 小嶋隆幸, 石丸哲, 辻川雅人, 白井正文, 高梨弘毅, 坂田修身, “硬 X 線を用いた新しいスピン分解光電子分光,” (28p DB-3), 日本物理学会 2013 年秋季大会, 徳島大学, (2013 年 9 月 28 日);
- [S. Ueda, M. Mizuguchi, T. Kojima, S. Ishimaru, M. Tsujikawa, M. Shirai, K. Takanashi, and O. Sakata, “New approach to spin-resolved photoemission using hard x-rays,” (28p DB-3),

Physical Society of Japan 2013 Autumn Meeting, Tokushima Univ., (28 September, 2013)].

[11] 辻川雅人, 白井正文, “MgO/FeCo 界面磁性の電界変調における界面格子歪みの効果,” (27a PS-20), 日本物理学会 第 69 回 年次大会, 東海大学, (2014 年 3 月 27 日);

[M. Tsujikawa and M. Shirai, “Role of lattice distortion in the electric-field control of magnetism at the MgO/FeCo interface,” (27a PS-20), Physical Society of Japan 69th Annual Meeting, Tokai Univ., (27 March, 2014)].

[12] 谷林慧, 三浦良雄, 白井正文, “ $Mn_{3-x}X_5Ga$  ( $X = Fe, Co, Ni$ ) の電子状態および MTJ の電気伝導特性,” (27a PS-33), 日本物理学会 第 69 回 年次大会, 東海大学, (2014 年 3 月 27 日);

[S. Tanibayashi, Y. Miura, and M. Shirai, “A first-principles study on the electronic structure of  $Mn_{3-x}X_5Ga$  ( $X = Fe, Co, Ni$ ) and the transport property of MTJ,” (27a PS-33), Physical Society of Japan 69th Annual Meeting, Tokai Univ., (27 March, 2014)].

[13] 水口将輝, 上田茂典, 三浦良雄, 小嶋隆幸, 白井正文, 高梨弘毅, “光電子分光による FeNi 規則合金薄膜の電子状態解析,” (30a AY-3), 日本物理学会 第 69 回 年次大会, 東海大学, (2014 年 3 月 30 日);

[M. Mizuguchi, S. Ueda, Y. Miura, T. Kojima, M. Shirai, K. Takanashi, “Study on electronic structures of FeNi ordered alloy thin films by photoelectron spectroscopy,” (30a AY-3), Physical Society of Japan 69th Annual Meeting, Tokai Univ., (30 March, 2014)].

(FY2014)

[1] 辻川雅人, 三浦良雄, 白井正文, “ $L1_0$ -FeNi 規則合金への軽元素添加効果の第一原理計算,” (5a C-4), 第 38 回 日本磁気学会 学術講演会, 慶応義塾大学, (2014 年 9 月 5 日);

[M. Tsujikawa, Y. Miura, and M. Shirai, “First principles study of light-element doping effects on  $L1_0$ -ordered FeNi,” (5a C-4), 38th Annual Conference on Magnetism in Japan, Keio Univ., (5 September, 2014)].

[2] 狩野駿, 辻川雅人, 阿部和多加, 白井正文, “磁気構造相変態を起こす Co 基ホイスラー合金の理論設計,” (7p PSA-92), 日本物理学会 2014 年秋季大会, 中部大学, (2014 年 9 月 7 日);

[S. Kano, M. Tsujikawa, K. Abe, and M. Shirai, “Theoretical design of Co-based Heusler alloys undergoing magnetostructural phase transformation,” (7p PSA-92), Physical Society of Japan 2014 Autumn Meeting, Chubu Univ., (7 September, 2014)].

[3] S. Kanai, M. Tsujikawa, M. Yamanouchi, S. Ikeda, Y. Miura, M. Shirai, F. Matsukura, and H. Ohno, “Magnetic anisotropy in Ta/CoFeB/MgO investigated by x-ray magnetic circular dichroism and first-principles calculation,” (17a S2-7), 2014 年 第 75 回 応用物理学会 秋季学術講演会, 北海道大学, (2014 年 9 月 17 日);

[75th JSAP Autumn Meeting 2014, Hokkaido Univ., (17 September, 2014)].

[4] K. Moges, Y. Honda, T. Uemura, M. Yamamoto, Y. Miura, and M. Shirai, “Effect of defects on the half-metallicity of quaternary Heusler alloy  $Co_2(Mn,Fe)Si$  thin films,” (A-21), 第 50 回 応用物理学会 北海道支部 / 第 11 回 日本光学会 北海道地区 合同学術講演会, 旭川市・勤労者福祉会館, (2015 年 1 月 10 日); [50th JSAP Hokkaido branch / 11th OSJ Hokkaido district Joint Meetings, Asahikawa, (10 January, 2015)].

[5] 三浦良雄, 辻川雅人, 白井正文, “Fe/MgO 接合における磁気緩和の電界効果の第一原理計算,” (11p P1-36), 2015 年 第 62 回 応用物理学会 春季学術講演会, 東海大学, (2015 年 3 月 11 日);

[Y. Miura, M. Tsujikawa, and M. Shirai, “*Ab initio* calculation of electric field effect on magnetic damping of Fe/MgO junctions,” (11p P1-36), 62nd JSAP Spring Meeting 2015, Tokai Univ., (11 March, 2015)].

[6] K. Moges, Y. Honda, T. Uemura, M. Yamamoto, Y. Miura, and M. Shirai, “Effect of off-stoichiometry on the half-metallic character of Heusler alloy  $Co_2(Mn,Fe)Si$  thin films,” (12a D11-5), 2015 年 第 62 回 応用物理学会 春季学術講演会, 東海大学, (2015 年 3 月 12 日); [62nd JSAP Spring Meeting 2015, Tokai Univ., (12 March, 2015)].

[7] 塩田明弘, 島田淳平, 関剛斎, 飯浜賢志, 水上成美, 辻川雅人, 白井正文, 高梨弘毅, “Ni/Co(111) 人工格子の磁気特性とダンピング定数,” (409), 日本金属学会 第 156 回 春季

講演大会, 東京大学, (2015年3月19日);

[A. Shiota, J. Shimada, T. Seki, S. Iihama, S. Mizukami, M. Tsujikawa, M. Shirai, and K. Takanashi, "Magnetic properties and magnetic damping constants of Ni/Co (111) superlattices," (409), 2015 Spring (156th) Meeting of JIM, Univ. of Tokyo, (19 March, 2015)].

[8] 阿部和多加, N. W. Ashcroft, "高密度水素の分子解離圧に対する非調和零点エネルギーの効果," (22a AC-10), 日本物理学会 第70回年次大会, 早稲田大学, (2015年3月22日);

[K. Abe and N. W. Ashcroft, "The effect of anharmonic zero-point energy on molecular dissociation pressure of dense hydrogen," (22a AC-10), Physical Society of Japan 70th Annual Meeting, Waseda Univ., (22 March, 2015)].

(FY2015)

[1] K. Moges, Y. Honda, H.-x. Liu, B. Hu, T. Uemura, Y. Miura, M. Shirai, and M. Yamamoto, "Effect of off-stoichiometry on the half-metallicity of quaternary Heusler alloy  $\text{Co}_2(\text{Mn,Fe})\text{Si}$  investigated through saturation magnetization and tunneling magnetoresistance," (11a A-7), 第39回 日本磁気学会 学術講演会, 名古屋大学, (2015年9月11日);

[39th Annual Conference on Magnetism in Japan, Nagoya Univ., (Sep. 11, 2015)].

[2] 相馬清吾, 本間康平, 菅原克明, 佐藤宇史, 辻川雅人, 白井正文, 高橋隆, "Fe(110)薄膜の表面電子バンド構造における酸素吸着効果: 高分解能 ARPES," (19a CG-2), 日本物理学会 2015年秋季大会, 関西大学, (2015年9月19日);

[S. Souma, K. Honma, K. Sugawara, T. Sato, M. Tsujikawa, M. Shirai, and T. Takahashi, "Effect of oxygen adsorption on surface electronic band structure of Fe(110) thin film," (19a CG-2), Physical Society of Japan 2015 Autumn Meeting, Kansai Univ., (19 September, 2015)].

[3] 岡林潤, 小山知弘, 鈴木基寛, 辻川雅人, 白井正文, 千葉大地, "Co/Cu/Ptの界面に誘起されたCuの垂直磁化の観測," (5B003), 第29回 日本放射光学学会 年会, 東京大学, (2016年1月11日);

[J. Okabayashi, T. Koyama, M. Suzuki, M. Tsujikawa, M. Shirai, and D. Chiba, "Observation of perpendicular magnetization induced at Cu in Co/Cu/Pt interface," Japanese Society for Synchrotron Radiation Research 29th Annual Meeting, Univ. of Tokyo, (11 January, 2016)].

[4] 伊藤啓太, 具志俊希, 東小蘭創真, 都甲薫, 白井正文, 角田匡清, 末益崇, "垂直磁気異方性をもつ正方晶フェリ磁性  $\text{Mn}_4\text{N}$  薄膜の磁気構造," (19p P1-17), 2016年 第63回 応用物理学会 春季学術講演会, 東京工業大学, (2016年3月19日);

[K. Ito, T. Gushi, S. Higashikozono, K. Toko, M. Shirai, M. Tsunoda, and T. Suemasu, "Magnetic structures of tetragonal ferrimagnetic  $\text{Mn}_4\text{N}$  films with perpendicular magnetic anisotropy," (19p P1-17), 63rd JSAP Spring Meeting 2016, Tokyo Institute of Technology, (19 March, 2016)].

[5] 梅津理恵, 齊藤耕太郎, 辻川雅人, 小野寛太, 石垣徹, 白井正文, " $\text{Mn}_2\text{CoGa}$  ホイスラ一合金の原子配列と電子状態," (19a PS-11), 日本物理学会 第71回 年次大会, 東北学院大学, (2016年3月19日);

[R. Y. Umetsu, K. Saito, M. Tsujikawa, K. Ono, T. Ishigaki, and M. Shirai, "Atomic arrangement and electronic state of  $\text{Mn}_2\text{CoGa}$  Heusler alloy," (19a PS-11), Physical Society of Japan 71st Annual Meeting, Tohoku Gakuin Univ., (19 March, 2016)].

[6] 阿部和多加, N. W. Ashcroft, "Bi及びSb水素化合物の高圧金属相," (19p BG-6) 日本物理学会 第71回年次大会, 東北学院大学, (2016年3月19日);

[K. Abe and N. W. Ashcroft, "Metallic phases in Bi and Sb hydrides at high pressures," (19p BG-6), Physical Society of Japan 71st Annual Meeting, Tohoku Gakuin Univ., (19 March, 2016)].

[7] 森川志門, 辻川雅人, 阿部和多加, 白井正文, " $\text{Co}_2\text{MnSi}/\text{Ag-Mg}/\text{Co}_2\text{MnSi}$  巨大磁気抵抗素子におけるスピン依存伝導の第一原理計算," (20p AU-2), 日本物理学会 第71回 年次大会, 東北学院大学, (2016年3月20日);

[S. Morikawa, M. Tsujikawa, K. Abe, and M. Shirai, "First-principles calculation of spin-dependent transport in  $\text{Co}_2\text{MnSi} / \text{Ag-Mg} / \text{Co}_2\text{MnSi}$  GMR devices," (20p AU-2), Physical Society of Japan 71st Annual Meeting, Tohoku Gakuin Univ., (20 March, 2016)].

[8] 田代敬之, 水口将輝, 小金澤智之, 三浦良雄, 辻川雅人, 白井正文, 鈴木英伸, 高梨弘

毅, “Ti 添加による  $L1_0$ -FeNi 規則合金薄膜の作製と評価,” (S1-11), 公募シンポジウム「永久磁石開発の元素戦略 4 –材料設計の新展開–」, 日本金属学会 第 158 回 2016 年春季講演大会, 東京理科大学, (2016 年 3 月 23 日);

[T. Y. Tashiro, M. Mizuguchi, T. Koganezawa, Y. Miura, M. Tsujikawa, M. Shirai, H. Suzuki, and K. Takanashi, “Fabrication and characterization of Ti-doped  $L1_0$ -FeNi ordered-alloy films,” (S1-11), Symposium: “Elements Strategy for the Development of Permanent Magnets 4: Frontiers in Materials Design,” 2016 Spring (158th) Meeting of JIM, Tokyo Univ. of Science, (23 March, 2016)].

(FY2016)

[1] 田代敬之, 水口将輝, 小金澤智之, 鈴木英伸, 三浦良雄, 辻川雅人, 白井正文, 高梨弘毅, “第三元素を添加した Fe/Ni 薄膜の規則化現象,” (5p E-1), 第 40 回 日本磁気学会 学術講演会, 金沢大学, (2016 年 9 月 5 日);

[T. Y. Tashiro, M. Mizuguchi, T. Koganezawa, H. Suzuki, Y. Miura, M. Tsujikawa, M. Shirai, and K. Takanashi, “Chemical ordering of Fe/Ni films doped with third-elements,” (5p E-1), 40th Annual Conference on Magnetism in Japan, Kanazawa Univ., (Sep. 5, 2016)].

[2] 関剛斎, 島田淳平, 飯浜賢志, 辻川雅人, 小金澤智之, 塩田明弘, 田代敬之, 周偉男, 菊池直登, 水上成美, 白井正文, 高梨弘毅, “Co/Ni エピタキシャル人工格子における磁気異方性とダンピング,” (5p E-2), 第 40 回 日本磁気学会 学術講演会, 金沢大学, (2016 年 9 月 5 日);

[T. Seki, J. Shimada, S. Iihama, M. Tsujikawa, T. Koganezawa, A. Shioda, T. Y. Tashiro, W. Zhou, N. Kikuchi, S. Mizukami, M. Shirai, and K. Takanashi, “Magnetic anisotropy and damping for Co/Ni epitaxial superlattices,” (5p E-2), 40th Annual Conference on Magnetism in Japan, Kanazawa Univ., (Sep. 5, 2016)].

[3] 辻川雅人, 白井正文, “5d 遷移金属単原子層による Fe および Co 表面における磁気異方性の電界変調増強,” (6a A-11), シンポジウム「Latest trends in ultra-low power consumption spintronic devices and circuits」, 第 40 回 日本磁気学会 学術講演会, 金沢大学, (2016 年 9 月 6 日);

[M. Tsujikawa and M. Shirai, “Enhancement of electric-field modulation of the magnetic anisotropy at Fe and Co surfaces covered by 5d transition-metal monolayer,” (6a A-11), 40th Annual Conference on Magnetism in Japan, Kanazawa Univ., (Sep. 6, 2016)].

[4] 田代敬之, 水口将輝, 小金澤智之, 鈴木英伸, 三浦良雄, 辻川雅人, 白井正文, 高梨弘毅, “[Fe-X/Ni] ( $X = \text{Ti, V}$ ) 多層膜の  $L1_0$  規則化,” (380), 日本金属学会 第 159 回 2016 年秋季講演大会, 大阪大学, (2016 年 9 月 23 日);

[T. Y. Tashiro, M. Mizuguchi, T. Koganezawa, H. Suzuki, Y. Miura, M. Tsujikawa, M. Shirai, and K. Takanashi, “ $L1_0$ -ordering of [Fe-X/Ni] ( $X = \text{Ti, V}$ ) multilayers,” (380), 2016 Fall (159th) Meeting of JIM, Osaka Univ., (23 September, 2016)].

[5] 関剛斎, 周偉男, 高梨弘毅, 島田淳平, 飯浜賢志, 田代敬之, 菊池直登, 辻川雅人, 白井正文, 水上成美, 小金澤智之, “原子層積層制御した Co/Ni エピタキシャル人工格子における磁気特性,” (382), 日本金属学会 第 159 回 2016 年秋季講演大会, 大阪大学, (2016 年 9 月 23 日);

[T. Seki, W. Zhou, K. Takanashi, J. Shimada, S. Iihama, T. Y. Tashiro, N. Kikuchi, M. Tsujikawa, M. Shirai, S. Mizukami, and T. Koganezawa, “Magnetic properties of atomic-layer deposited Co/Ni epitaxial superlattices,” (382), 2016 Fall (159th) Meeting of JIM, Osaka Univ., (23 September, 2016)].

[6] 水口将輝, 高梨弘毅, 堀田善治, 白井正文, 小嗣真人, “ $L1_0$  型 FeNi 規則合金の作製と評価,” (MAG-16-194), 電気学会 マグネティクス研究会「永久磁石と応用」, 日本電気計器検定所, (2016 年 11 月 29 日);

[M. Mizuguchi, K. Takanashi, Z. Horita, M. Shirai, and M. Kotsugi, “Fabrication and characterization of  $L1_0$ -type FeNi ordered alloy,” (MAG-16-194), IEEJ Magnetism Society Meeting, Japan Electric Meters Inspection Corporation, Tokyo, (29 November, 2016)].

[7] 嶋敏之, 土井正晶, 岡田宏成, 熊谷直也, 高橋啓一, 辻川雅人, 白井正文, “ラティスエンジニアリングによる高磁化磁性材料の創製ならびに革新的永久磁石材料の開発,” (MAG-16-196), 電気学会 マグネティクス研究会「永久磁石と応用」, 日本電気計器検

定所, (2016年11月29日);

[T. Shima, M. Doi, H. Okada, N. Kumagai, K. Takahashi, M. Tsujikawa, and M. Shirai, "Development of novel magnetic materials through lattice engineering," (MAG-16-196), IEEJ Magnetics Society Meeting, Japan Electric Meters Inspection Corporation, Tokyo, (29 November, 2016)].

[8] 角田一樹, 辻川雅人, 許焜, 上田茂典, 陳家華, 朱思源, 白井正文, 貝沼亮介, 木村昭夫, "硬 X 線光電子分光によるホイスラー合金  $\text{Co}_2\text{Cr}(\text{Ga},\text{Si})$  の電子状態の研究," (3B001), 第 30 回 日本放射光学会 年会・放射光科学合同シンポジウム, 神戸芸術センター, (2017年1月8日);

[K. Sumida, M. Tsujikawa, X. Xu, S. Ueda, J. Chen, S. Zhu, M. Shirai, R. Kainuma, and A. Kimura, "Study on electronic states of  $\text{Co}_2\text{Cr}(\text{Ga},\text{Si})$  Heusler alloys by using hard x-ray photoelectron spectroscopy," (3B001), Japanese Society for Synchrotron Radiation Research 30th Annual Meeting, Kobe, (8 January, 2017)].

[9] 隈田壮, 辻川雅人, 白井正文, "CoFe<sub>3</sub>N/BaTiO<sub>3</sub> 接合界面における電気分極反転に伴う巨大な磁気モーメント変化," (14p P10-59), 2017年 第64回 応用物理学会 春季学術講演会, パシフィコ横浜, (2017年3月14日);

[S. Kumata, M. Tsujikawa, and M. Shirai, "Huge magnetic-moment variation at  $\text{CoFe}_3\text{N}/\text{BaTiO}_3$  interfaces induced by electric-polarization reversal," (14p P10-59), 64th JSAP Spring Meeting 2017, Pacifico Yokohama, (14 March, 2017)].

[10] 辻川雅人, 白井正文, "典型元素を添加した Mn-Ga 合金の磁気特性に関する第一原理計算," (17a C36-7), 日本物理学会 第72回 年次大会, 大阪大学, (2017年3月17日);

[M. Tsujikawa and M. Shirai, "A first-principles study on magnetic properties of typical-element doped Mn-Ga alloys," (17a C36-7), Physical Society of Japan 72nd Annual Meeting, Osaka Univ., (17 March, 2017)].

[11] 今諒磨, 辻川雅人, 阿部和多加, 白井正文, "Co 基ホイスラー合金における磁気構造相転移の物性発現に関する理論研究," (17a K-PS-47), 日本物理学会 第72回 年次大会, 大阪大学, (2017年3月17日);

[R. Kon, M. Tsujikawa, K. Abe, and M. Shirai, "Theoretical study of physical origin of magnetostructural phase transition in Co-based Heusler alloys," (17a K-PS-47), Physical Society of Japan 72nd Annual Meeting, Osaka Univ., (17 March, 2017)].

[12] 阿部和多加, "スカンジウム水素化合物の高圧金属相," (18a C21-7), 日本物理学会 第72回年次大会, 大阪大学, (2017年3月18日);

[K. Abe, "Metallic phases of Sc hydrides at high pressures," (18a C21-7), Physical Society of Japan 72nd Annual Meeting, Osaka Univ., (18 March, 2017)].

(FY2017)

[1] 角田一樹, 辻川雅人, 許焜, 陳家華, 朱思源, 吉川智己, 檜垣聡太, 上田茂典, 竹田幸治, 斎藤祐児, 白井正文, 貝沼亮介, 木村昭夫, "放射光分光および第一原理計算を用いたホイスラー合金  $\text{Co}_2\text{Cr}(\text{Ga},\text{Si})$  のリエントラント・マルテンサイト変態," (S6.20), シンポジウム S6 「分野融合による機能性ホイスラー合金材料研究の新展開」, 日本金属学会 第161回 2017年秋季講演大会, 北海道大学, (2017年9月8日);

[K. Sumida, M. Tsujikawa, X. Xu, J. Chen, S. Zhu, T. Yoshikawa, S. Higaki, S. Ueda, Y. Takeda, Y. Saitoh, M. Shirai, R. Kainuma, and A. Kimura, "Reentrant martensitic transformation in Heusler alloys  $\text{Co}_2\text{Cr}(\text{Ga},\text{Si})$  revealed by synchrotron radiation spectroscopy and first-principles calculation," (S6.20), Symposium S6: "Frontiers in investigations of functional Heusler alloys by field fusion," 2017 Fall (161st) Meeting of JIM, Hokkaido Univ., (8 September, 2017)].

[2] M. Tsujikawa and M. Shirai, "The effect of Os or Ir layer insertion into MgO/Fe interface on the electric-field modulation of magnetic anisotropy," (19p D-6), Symposium on "Controlling magnetization by applying electric current and voltage," 第41回 日本磁気学会 学術講演会, 九州大学, (2017年9月19日);

[41st Annual Conference on Magnetics in Japan, Kyushu Univ., (Sep. 19, 2017)].

[3] 金村卓郎, 白井正文, "機械学習による遷移金属二元合金の磁化予測," (19p A-12), 第41回 日本磁気学会 学術講演会, 九州大学, (2017年9月19日);

- [T. Kanemura and M. Shirai, "Prediction of the magnetization in transition-metal binary alloys by means of machine learning," (19p A-12), 41st Annual Conference on Magnetism in Japan, Kyushu Univ., (Sep. 19, 2017)].
- [4] 三橋唯澄, 辻川雅人, 白井正文, "格子拡張による高磁化 Mn 基規則合金の理論設計," (19p A-13), 第 41 回 日本磁気学会 学術講演会, 九州大学, (2017 年 9 月 19 日); [Y. Mitsuhashi, M. Tsujikawa, and M. Shirai, "Theoretical design of Mn-based ordered alloys with high magnetization by lattice expansion," (19p A-13), 41st Annual Conference on Magnetism in Japan, Kyushu Univ., (Sep. 19, 2017)].
- [5] 角田一樹, 辻川雅人, 許焜, 陳家華, 朱思源, 吉川智己, 檜垣聡太, 上田茂典, 竹田幸治, 斎藤祐児, 白井正文, 貝沼亮介, 木村昭夫, "ホイスラー合金  $\text{Co}_2\text{Cr}(\text{Ga},\text{Si})$  におけるリエントラント・マルテンサイト変態機構," (23p PSA-4), 日本物理学会 2017 年秋季大会, 岩手大学, (2017 年 9 月 23 日); [K. Sumida, M. Tsujikawa, X. Xu, J. Chen, S. Zhu, T. Yoshikawa, S. Higaki, S. Ueda, Y. Takeda, Y. Saitoh, M. Shirai, R. Kainuma, and A. Kimura, "Mechanism of reentrant martensitic transformation in Heusler alloys  $\text{Co}_2\text{Cr}(\text{Ga},\text{Si})$ ," (23p PSA-4), Physical Society of Japan 2017 Autumn Meeting, Iwate Univ., (23 September, 2017)].
- [6] L. Bainsla, K. Z. Suzuki, M. Tsujikawa, H. Tsuchiura, M. Shirai, and S. Mizukami, "Magnetic tunnel junctions with an equiatomic  $\text{CoFeMnSi}$  Heusler alloy electrode," (17p P10-34), 2018 年 第 65 回 応用物理学会 春季学術講演会, 早稲田大学, (2018 年 3 月 17 日); [65th JSAP Spring Meeting 2018, Waseda Univ., (17 March, 2018)].
- [7] Y. Jibiki, M. Goto, M. Tsujikawa, Philipp Risius, K. Nawaoka, M. Shirai, S. Miwa, and Y. Suzuki, "Influence of surface resonant state on voltage-controlled magnetic anisotropy," (17p P10-80), 2018 年 第 65 回 応用物理学会 春季学術講演会, 早稲田大学, (2018 年 3 月 17 日); [65th JSAP Spring Meeting 2018, Waseda Univ., (17 March, 2018)].
- [8] T. Kawabe, K. Yoshikawa, M. Tsujikawa, T. Tsukahara, K. Nawaoka, Y. Kotani, K. Toyoki, M. Goto, M. Suzuki, T. Nakamura, M. Shirai, Y. Suzuki, and S. Miwa, "Bruno mechanism on voltage-controlled magnetic anisotropy in ultrathin cobalt films," (19a D104-2), 2018 年 第 65 回 応用物理学会 春季学術講演会, 早稲田大学, (2018 年 3 月 19 日); [65th JSAP Spring Meeting 2018, Waseda Univ., (19 March, 2018)].
- [9] T. Nozaki, A. Koziol-Rachwal, M. Tsujikawa, Y. Shiota, X. Xu, T. Yamamoto, T. Ohkubo, T. Tsukahara, S. Miwa, M. Suzuki, S. Tamaru, H. Kubota, A. Fukushima, K. Hono, M. Shirai, Y. Suzuki, and S. Yuasa, "Enhancement interfacial perpendicular magnetic anisotropy and voltage-controlled magnetic anisotropy in iridium-doped  $\text{Fe}/\text{MgO}$  structures," (19a D104-4), 2018 年 第 65 回 応用物理学会 春季学術講演会, 早稲田大学, (2018 年 3 月 19 日); [65th JSAP Spring Meeting 2018, Waseda Univ., (19 March, 2018)].
- [10] 相馬清吾, 本間康平, 佐藤宇史, 辻川雅人, 白井正文, 高橋隆, "Fe(110)薄膜の表面電子バンド構造における酸素吸着効果: 高分解能 ARPES," (19p F214-4), 2018 年 第 65 回 応用物理学会 春季学術講演会, 早稲田大学, (2018 年 3 月 19 日); [S. Souma, K. Honma, T. Sato, M. Tsujikawa, M. Shirai, and T. Takahashi, "Oxygen adsorption effect on surface electronic band structure in Fe(110) thin film: High-resolution ARPES," (19p F214-4), 65th JSAP Spring Meeting 2018, Waseda Univ., (19 March, 2018)].
- [11] 阿部和多加, "高密度ジルコニウム水素化合物の第一原理構造探索," (23p B401-8), 日本物理学会 第 73 回年次大会, 東京理科大学, (2018 年 3 月 23 日); [K. Abe, "First-principles structural exploration of dense Zr hydrides," (23p B401-8), Physical Society of Japan 73rd Annual Meeting, Tokyo Univ. of Science, (23 March, 2018)].
- [12] 河辺健志, 吉川晃平, 辻川雅人, 塚原拓也, 繩岡孝平, 小谷佳範, 豊木研太郎, 後藤穰, 鈴木基寛, 中村哲也, 白井正文, 鈴木義茂, 三輪真嗣, "Co/MgO 多層膜における磁気モーメント及び磁気異方性の電圧変調," (23p K304-10), 日本物理学会 第 73 回 年次大会, 東京理科大学, (2018 年 3 月 23 日); [T. Kawabe, K. Yoshikawa, M. Tsujikawa, T. Tsukahara, K. Nawaoka, Y. Kotani, K. Toyoki, M. Goto, M. Suzuki, T. Nakamura, M. Shirai, Y. Suzuki, and S. Miwa, "Electric-field-induced changes in magnetic moments and magnetic anisotropy in Co/MgO multilayer," (23p K304-10), Physical Society of Japan 73rd Annual Meeting, Tokyo Univ. of Science, (23 March, 2018)].

[13]相馬清吾, 本間康平, 佐藤宇史, 辻川雅人, 白井正文, 高橋隆, “酸素吸着 Fe(110)表面の高分解能 ARPES,” (24p K402-2), 日本物理学会 第 73 回 年次大会, 東京理科大学, (2018 年 3 月 24 日);

[S. Souma, K. Honma, T. Sato, M. Tsujikawa, M. Shirai, and T. Takahashi, “High-resolution ARPES of oxygen-adsorbed Fe(110) surface,” (24p K402-2), Physical Society of Japan 73rd Annual Meeting, Tokyo Univ. of Science, (24 March, 2018)].

[14]鹿子木将明, 角田一樹, 許晶, 辻川雅人, 白井正文, 奥田太一, 貝沼亮介, 木村昭夫, “高分解能光電子分光による Co 基ホイスラー型形状記憶合金の電子状態,” (24p K402-4), 日本物理学会 第 73 回 年次大会, 東京理科大学, (2018 年 3 月 24 日);

[M. Kakoki, K. Sumida, X. Xu, M. Tsujikawa, M. Shirai, T. Okuda, R. Kainuma, and A. Kimura, “Electronic structure of Co-based shape memory Heusler alloys revealed by high-resolution photoemission spectroscopy,” (24p K402-4), Physical Society of Japan 73rd Annual Meeting, Tokyo Univ. of Science, (24 March, 2018)].

(FY2018)

[1] 金村卓郎, Tufan Roy, 辻川雅人, 白井正文, “機械学習を用いた四元ホイスラー合金の物性予測,” (18p PB1-34), 2018 年 第 79 回 応用物理学会 秋季学術講演会, 名古屋国際会議場, (2018 年 9 月 18 日);

[T. Kanemura, T. Roy, M. Tujikawa, and M. Shirai, “Prediction of physical properties of quaternary Heusler alloys using machine learning,” (18p PB1-34), 79th JSAP Autumn Meeting 2018, Nagoya Congress Center, (18 September, 2018)].

[2] T. Tsuchiya, L. Bainsla, T. Roy, K. Elphick, M. Tsujikawa, M. Shirai, A. Hirohata, and S. Mizukami, “Magnetic properties and magnetic tunnel junctions of equiatomic quaternary CoFeCrAl Heusler alloy epitaxial films,” (18p PB1-35), 2018 年 第 79 回 応用物理学会 秋季学術講演会, 名古屋国際会議場, (2018 年 9 月 18 日);

[79th JSAP Autumn Meeting 2018, Nagoya Congress Center, (18 September, 2018)].

[3] R. Okado, M. Tsujikawa, and M. Shirai, “The magnetic anisotropy of the Co films on ZnO with Zn- and O-terminated interfaces,” (18p PB1-44), 2018 年 第 79 回 応用物理学会 秋季学術講演会, 名古屋国際会議場, (2018 年 9 月 18 日);

[79th JSAP Autumn Meeting 2018, Nagoya Congress Center, (18 September, 2018)].

[4] M. Tsujikawa and M. Shirai, “Effect of lattice distortion on voltage-controlled magnetic anisotropy at MgO/FeCo interface,” (20p 131-8), 2018 年 第 79 回 応用物理学会 秋季学術講演会, 名古屋国際会議場, (2018 年 9 月 20 日);

[79th JSAP Autumn Meeting 2018, Nagoya Congress Center, (20 September, 2018)].

[5] 前野央, 柳瀬隆, 島田敏宏, 辻川雅人, 白井正文, 長浜太郎, “ $D0_{19}$  型  $X_3\text{Sn}$  ( $X = \text{Fe}, \text{Mn}$ ) 薄膜の作製とその磁気伝導特性,” (9p PB1-16), 2019 年 第 66 回 応用物理学会 春季学術講演会, 東京工業大学, (2019 年 3 月 9 日);

[A. Maeno, T. Yanase, T. Shimada, M. Tsujikawa, M. Shirai, and T. Nagahama, “Fabrication of  $D0_{19}$ - $X_3\text{Sn}$  ( $X = \text{Fe}, \text{Mn}$ ) thin films and their magnetotransport properties,” (9p PB1-16), 66th JSAP Spring Meeting 2019, Tokyo Institute of Technology, (9 March, 2019)].

(7) 査読なし国内研究会・講演会 / Presentations in domestic conferences

該当なし N/A

(8) 著書 / Books

該当なし N/A

(9) 特許 / Patents

(FY2016)

[1]  $L1_0$  型 FeNi 規則合金の製造方法

特願 2016-175873 号 (出願日: 2016 年 9 月 8 日)

特開 2018-41873 号 (公開日 : 2018 年 3 月 15 日)  
(発明者) 水口将輝, 田代敬之, 高梨弘毅, 三浦良雄, 辻川雅人, 白井正文  
(出願人) 国立大学法人 東北大学

Title of Invention: Fabrication method of L1<sub>0</sub>-type FeNi ordered alloy  
Application Number: 特願 2016-175873 (Application Date: 8 September, 2016)  
Filing Number: 特開 2018-41873 (Filing Date: 15 March, 2018)  
Inventors: Masaki Mizuguchi, Takayuki Tashiro, Koki Takanashi, Yoshio Miura,  
Masahito Tsujikawa, Masafumi Shirai  
Patentee: Tohoku University

[2] 磁性薄膜及び磁性薄膜の製造方法

特願 2016-245883 号 (出願日 : 2016 年 12 月 19 日)  
特開 2018-101673 号 (公開日 : 2018 年 6 月 28 日)  
(発明者) 関 剛斎, 高梨弘毅, 辻川雅人, 白井正文  
(出願人) 国立大学法人 東北大学

Title of Invention: Magnetic films and fabrication method of the magnetic films  
Application Number: 特願 2016-245883 (Application Date: 19 December, 2016)  
Filing Number: 特開 2018-101673 (Filing Date: 28 June, 2018)  
Inventors: Takeshi Seki, Koki Takanashi, Masahito Tsujikawa, Masafumi Shirai  
Patentee: Tohoku University

(FY2017)

[1] 磁気素子、磁気記憶装置及び磁気センサ

特願 2017-067235 号 (出願日 : 2017 年 3 月 30 日)  
PCT/JP2018/5290 (出願日 : 2018 年 2 月 15 日)  
(発明者) 野崎隆行, 湯浅新治, コジオルラフバン アナ, 辻川雅人, 白井正文,  
宝野和博, 大久保忠勝, 徐 先東  
(出願人) 国立研究開発法人 産業技術総合研究所,  
国立大学法人 東北大学,  
国立研究開発法人 物質・材料研究機構

Title of Invention: Magnetic device, magnetic recording system, and magnetic sensor  
Application Number: 特願 2017-067235 (Application Date: 30 March, 2017)  
Application Number: PCT/JP2018/5290 (Application Date: 15 February, 2018)  
Inventors: Takayuki Nozaki, Shinji Yuasa, Anna Koziol-Rachwal, Masahito Tsujikawa,  
Masafumi Shirai, Kazuhiro Hono, Tadakatsu Ohkubo, Xiandong Xu  
Patentees: National Institute of Advanced Industrial Science and Technology,  
Tohoku University, National Institute for Materials Science

(10) 招待講演 / Invited Talks

(FY2013)

[1] M. Shirai, M. Tsujikawa, and Y. Miura, "First-principles study on magneto-crystalline anisotropy at Co-Fe-Al/MgO interfaces," JSPS York-Tohoku Symposium on Magnetic Materials and Spintronic Devices, York, UK, (10-12 June, 2013).

[2] M. Shirai, M. Tsujikawa, and Y. Miura, "Ab initio study on magneto-crystalline anisotropy in Co-Fe/MgO junctions," International Workshop of Computational Nano-Materials Design on Green Energy, Joint Workshop of Interactive Materials Science Cadet Program, Osaka University and JSPS Core-to-Core Program (A) Advanced Research Network, Awaji, Japan, (16-19 June, 2013).

[3] Y. Miura, M. Tsujikawa, and M. Shirai, "A first-principles study on magneto-crystalline anisotropy at interfaces of Fe with various non-magnetic metals," International Workshop



of Computational Nano-Materials Design on Green Energy, Joint Workshop of Interactive Materials Science Cadet Program, Osaka University and JSPS Core-to-Core Program (A) Advanced Research Network, Awaji, Japan, (16-19 June, 2013).

[4] M. Shirai, Y. Miura, S. Ozaki, Y. Kuwahara, M. Tsujikawa, and K. Abe, "First-principles calculations of magneto-crystalline anisotropy in  $L1_0$ -ordered FeNi and Fe/Ni multilayers," Symposium on "Elements strategy initiative for permanent magnets," 第 37 回 日本磁気学会 学術講演会, 北海道大学, (2013 年 9 月 5 日);

[37th Annual Conference on Magnetism in Japan, Hokkaido Univ., (5 September, 2013)].

(FY2014)

[1] M. Shirai, "Magneto-crystalline anisotropy of  $L1_0$ -ordered FeNi alloy: A first-principles study," US-Japan Bilateral 1st Meeting on Rare Metals, Tsukuba, Japan, (20 May, 2014).

[2] Y. Miura, S. Tanibayashi, and M. Shirai, "A first-principles study on electronic structures and transport properties of magnetic tunnel junctions with  $D0_{22}$ -type Mn-based tetragonal Heusler alloys," International Workshop of Computational Nano-Materials Design on Green Energy, Joint Workshop of Center of Asia Research and Education Network, Osaka University and JSPS Core-to-Core Program (A) Advanced Research Network, Toyonaka, Japan, (1-3 June, 2014).

[3] M. Tsujikawa and M. Shirai, "Electric-field control of the perpendicular magnetic anisotropy at ferromagnet/oxide interfaces: A first-principles study," International Workshop of Computational Nano-Materials Design on Green Energy, Joint Workshop of Center of Asia Research and Education Network, Osaka University and JSPS Core-to-Core Program (A) Advanced Research Network, Toyonaka, Japan, (1-3 June, 2014).

[4] M. Shirai, "First-principles study on electric-field modulation of interfacial magnetic anisotropy," 2nd Japan-EU Open Workshop on Heusler Alloy Replacement for Iridium, Sendai, Japan, (12 September, 2014).

(FY2015)

[1] M. Shirai, "Theoretical design of electrode materials for magnetic tunnel junctions with MgO barrier: Ferrimagnetic  $D0_{22}$ -type Mn-based Heusler alloys," York-Tohoku-Kaiserslautern Symposium on New-Concept Spintronics Devices, including Core-to-Core Kick-Off Meeting, Sir Martin Wood Prize Lecture and the 3rd HARFIR Open Workshop, York, UK, (11-13 June, 2015).

[2] M. Shirai, "Fundamental knowledge of first-principles calculation," (11p A-2), Symposium on "Tutorial symposium on theoretical calculation and computer physics in magnetism and magnetism," 第 39 回 日本磁気学会 学術講演会, 名古屋大学, (2015 年 9 月 11 日);

[39th Annual Conference on Magnetism in Japan, Nagoya Univ., (11 September, 2015)].

[3] 白井正文, "ホイスラー合金磁気抵抗素子の界面の電子論," (S4-5), シンポジウム「機能性ホイスラー合金研究の最先端」, 日本金属学会 第 157 回 秋季講演大会, 九州大学, (2015 年 9 月 17 日);

[M. Shirai, "Electronic structure at interface of magnetoresistance devices composed of Heusler alloys," (S4-5), Symposium: "Frontiers in investigations of functional Heusler alloys," 2015 Fall (157th) Meeting of JIM, Kyushu Univ., (17 September, 2015)].

[4] M. Shirai, "Electronic structure at interfaces between Heusler alloys and MgO." Tohoku Forum of Creativity International Workshop: Spintronics, 13th RIEC International Workshop on Spintronics, Sendai, Japan, (18-20 November, 2015).

[5] M. Shirai, "*Ab initio* study on magnetic tunnel junctions using Heusler alloys," International Workshop on Computational Nano-Materials Design and Realization for Energy-Saving and Energy-Creation Materials, Toyonaka, Japan, (25-26 March, 2016).

(FY2016)

[1] S. Miwa, M. Suzuki, M. Tsujikawa, K. Matsuda, T. Nozaki, K. Tanaka, M. Goto, Y. Kotani, T. Ohkubo, F. Bonell, E. Tamura, K. Hono, T. Nakamura, M. Shirai, and Y. Suzuki, "Voltage

control of platinum orbit: Contribution to interfacial magnetic anisotropy change,” 61st Annual Conference on Magnetism and Magnetic Materials, New Orleans, Louisiana, USA, (31 October - 4 November, 2016).

[2] M. Shirai, “Enhancement of voltage-controlled magnetic anisotropy by 5d transition-metal monolayer on ferromagnetic thin films,” Spintronics and Core-to-Core Workshop 2017, Osaka, Japan, (20-22 March, 2017).

[3] 白井正文, “スピントロニクス実用材料の理解と高性能スピン伝導デバイスの設計,” (16p 501-4), シンポジウム「スピン伝導デバイスの進展と応用の最前線」, 2017年 第64回 応用物理学会 春季学術講演会, パシフィコ横浜, (2017年3月16日);

[M. Shirai, “Insight into materials for spintronics applications and design of high-performance spin-dependent transport devices,” (16p 501-4), Symposium: “Frontiers in development and applications of spin-transport devices,” 64th JSAP Spring Meeting 2017, Pacifico Yokohama, (16 March, 2017)].

(FY2017)

[1] M. Shirai, “Enhancement of voltage effect on magnetic anisotropy in ferromagnetic thin films,” York-Tohoku-Kaiserslautern Research Symposium on “New-Concept Spintronics Devices”, York, UK, (21-23 June, 2017).

[2] T. Nozaki, Y. Shiota, A. Koziol-Rachwal, M. Tsujikawa, X. Xu, T. Ohkubo, T. Tsukahara, S. Miwa, M. Suzuki, S. Tamaru, H. Kubota, A. Fukushima, K. Hono, M. Shirai, and Y. Suzuki, “Recent progress in voltage-controlled magnetic anisotropy –Towards the realization of voltage-torque MRAM–,” 28th Magnetic Recording Conference, Tsukuba, Japan, (2-4 August, 2017).

[3] T. Nozaki, Y. Shiota, A. Koziol-Rachwal, M. Tsujikawa, T. Yamamoto, X. Xu, T. Ohkubo, T. Tsukahara, S. Miwa, M. Suzuki, S. Tamaru, H. Kubota, A. Fukushima, K. Hono, M. Shirai, S. Yuasa, and Y. Suzuki, “Recent progress and future challenges in voltage-controlled magnetic anisotropy,” (19p D-4), Symposium on “Controlling magnetization by applying electric current and voltage,” 第41回 日本磁気学会 学術講演会, 九州大学, (2017年9月19日); [41st Annual Conference on Magnetism in Japan, Kyushu Univ., (19 September, 2017)].

[4] T. Shima, M. Doi, H. Okada, M. Tsujikawa, and M. Shirai, “Development of Mn-based novel magnetic materials through lattice engineering,” (20a C-1), Symposium on “High performance magnets and evaluation techniques toward innovative development for next generation magnets,” 第41回 日本磁気学会 学術講演会, 九州大学, (2017年9月20日); [41st Annual Conference on Magnetism in Japan, Kyushu Univ., (20 September, 2017)].

[5] S. Miwa, K. Nawaoka, J. Cho, T. Nozaki, M. Suzuki, M. Tsujikawa, M. Goto, F. Bonell, E. Tamura, H. Kubota, S. Tamaru, K. Yakushiji, A. Fukushima, Y. Kotani, T. Nakamura, M. Shirai, T. Ohkubo, K. Hono, C.-Y. You, S. Yuasa, and Y. Suzuki, “Voltage control of interfacial magnetic anisotropy, Dzyaloshinskii-Moriya interaction and exchange coupling in Fe/MgO-based artificial multilayers,” 2017 MRS Fall Meeting & Exhibit, Symposium EM2 – Multiferroics and Magnetoelectrics, Boston, Massachusetts, USA, (26 November - 1 December, 2017).

[6] M. Shirai, “Enhancement of voltage-controlled magnetic anisotropy by Ir insertion into Fe/MgO interface,” International Workshop on New Excitations in Spintronics, Sendai, Japan, (10-12 January, 2018).

(FY2018)

[1] T. Nozaki, A. Koziol-Rachwal, M. Tsujikawa, Y. Shiota, T. Yamamoto, T. Ikeura, X. Xu, T. Ohkubo, T. Tsukahara, S. Miwa, M. Suzuki, H. Imamura, S. Tamaru, H. Kubota, A. Fukushima, K. Hono, M. Shirai, Y. Suzuki, and S. Yuasa, “Very large voltage-controlled magnetic anisotropy and extremely reliable voltage-induced switching,” Intermag 2018, Singapore, (23-27 April, 2018).

[2] R. Y. Umetsu, X. Xu, W. Ito, M. Tsujikawa, M. Shirai, and R. Kainuma, “Change in the density of states during the martensitic phase transformation for NiMn-based metamagnetic shape memory alloys,” International Conference on Processing and

Manufacturing of Advanced Materials, Processing, Fabrication, Properties, Applications, Paris, France, (9-13 July, 2018).

[3] M. Suzuki, M. Tsujikawa, T. Nozaki, T. Nakamura, M. Shirai, S. Yuasa, Y. Suzuki, and S. Miwa, "Microscopic mechanism of the electric-field effects on spintronic devices elucidated by x-ray magnetic dichroism spectroscopy," International Conference on Solid State Devices and Materials (SSDM 2018), Tokyo, Japan, (9-13 September, 2018).

[4] S. Yuasa, T. Nozaki, T. Yamamoto, M. Tsujikawa, and M. Shirai, "Voltage control of magnetic anisotropy and its application to voltage-torque MRAM," Symposium on Topological Phases and Functionality of Correlated Electron Systems (TPFC 2019), Kashiwa, Japan, (18-20 February, 2019).

[5] M. Shirai, "Enhancement of voltage-controlled magnetic anisotropy in Fe/MgO junctions by inserting heavy elements," 2nd Tohoku/SG-Spin Workshop on Spintronics, Singapore, (22-23 February, 2019).

## 2. 学会活動 / Activities in academic societies

### (1) 学会役員等の活動 / Activities on committees of academic societies

該当なし N/A

### (2) 学術的国際会議の企画・運営

Planning and organizing academic international conferences.

(FY 2013)

[1] M. Shirai, a member of Organizing and Local Committee, International Workshop of Computational Nano-Materials Design on Green Energy, Awaji, Japan (16-19 June, 2013).

(FY2014)

[2] M. Shirai, a member of Organizing Committee, International Workshop of Computational Nano-Materials Design on Green Energy, Toyonaka, Japan (1-3 June, 2014).

(FY2015)

[3] M. Shirai, a member of Organizing Committee, International Workshop of Computational Nano-Materials Design and Realization for Energy-Saving and Energy-Creation Materials, Toyonaka, Japan (25-26 March, 2016).

(FY2016)

[4] M. Shirai, a member of Organizing Committee, EU-Japan Workshop on Computational Materials Design and Realization for Spintronics, Moltronics, Quantronics, Superconductivity and Topotronics, Jülich, Germany (18-30 September, 2016).

[5] M. Shirai, a member of Organizing and Local Committee, 14th RIEC International Workshop on Spintronics, Sendai, Japan (17-19 November, 2016).

(FY2017)

[6] M. Shirai, a member of Program Committee, Kick-off Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan (19-20 February, 2018).

(FY2018)

[7] M. Shirai, a member of Organizing Committee, 8th JSPS Core-to-Core Workshop on “New-Concept Spintronic Devices”, Sendai, Japan (11-12 January, 2019).

[8] M. Shirai, a member of Organizing Committee, 2nd Symposium for World Leading Research Centers – Materials Science and Spintronics –, Sendai, Japan (16-18 February, 2019).

[9] M. Shirai, a member of Organizing Committee, 2nd Tohoku/SG-Spin Workshop on Spintronics, Singapore (22-23 February, 2019).

(3) 学術論文誌の編集・査読 / Editor and reviewer for academic journals.

該当なし N/A

### 3. 社会貢献 / Contributions to society

(1) 教育活動 / Educational activities outside university

[1] 白井正文, 第 36 回 応用磁気学会サマースクール 講師 (2013 年 7 月 17 日).

Masafumi Shirai, a lecturer, 36th Summer School, the Magnetism Society of Japan, (17 July, 2013).

[2] 白井正文, 応用物理学会スピントロニクス研究会主催

第 13 回 スピントロニクス入門セミナー 講師 (2014 年 10 月 27 日~29 日).

Masafumi Shirai, a lecturer, 13th School on Spintronics, Professional Group of Spintronics, the Japan Society of Applied Physics, (27-29 October, 2014).

[3] 白井正文, 日本物理学会 Jr.セッション委員会委員 (2015 年 4 月~).

Masafumi Shirai, a member of Jr. Session Committee, the Physical Society of Japan, (April 2015 -).

[4] 白井正文, コンピュータショナル・マテリアルズ・デザイン・ワークショップ 講師, 大阪大学, 第 28 回 (2016 年 3 月 4 日~8 日); 第 29 回 (2016 年 9 月 5 日~9 日); 第 30 回 (2017 年 2 月 27 日~3 月 3 日); 第 31 回 (2017 年 9 月 11 日~15 日); 第 32 回 (2018 年 2 月 26 日~3 月 2 日); 第 33 回 (2018 年 9 月 3 日~7 日); 第 34 回 (2019 年 2 月 18 日~22 日).

Masafumi Shirai, a lecturer, Computational Materials Design (CMD) Workshop, Osaka University, 28th (29 February - 4 March, 2016); 29th (5-9 September, 2016); 30th (27 February - 3 March, 2017); 31st (11-15 September, 2017); 32nd (26 February - 2 March, 2018); 33rd (3-7 September, 2018); 34th (18-22 February, 2019).

[5] 白井正文, 名古屋大学大学院工学研究科 非常勤講師 (2017 年 11 月 15 日~17 日).

Masafumi Shirai, a part-time lecturer, Graduate School of Engineering, Nagoya University, (15-17 November, 2017).

(2) 産業界における指導・啓蒙 / Instruction and education for industry

[1] 白井正文, 辻川雅人, 学術指導「交換相互作用  $J$  の算出に関する指導」, 住友金属鉱山株式会社 (2016 年度~2017 年度).

Masafumi Shirai and Masahito Tsujikawa, Academic instruction on "Evaluation of exchange interaction *J*," Sumitomo Metal Mining Co., Ltd. (FY2016 - FY2017).

(3) 国・地方自治体・公共団体における活動

Activities for national and local governments, and public organizations

[1] 白井正文, 日本学術振興会 (JSPS) 研究開発専門委員会委員 (幹事),  
「産業応用をめざした新物質機能の設計と実証」(2011年10月~2014年9月).

Masafumi Shirai, a member (secretary), Expert Committee for Research and Development  
"Design and demonstration of new materials functionality for industrial applications,"  
Japanese Society for the Promotion of Science (JSPS), (October 2011 - September 2014).

[1] 白井正文, 日本学術振興会 (JSPS) 特別研究員等審査会専門委員,  
(2014年8月~2016年7月).

Masafumi Shirai, an expert advisor, Screening Committee of Research Fellowship for  
Young Scientists, Japanese Society for the Promotion of Science (JSPS), (August 2014 -  
July 2016).

[2] 白井正文, 日本学術振興会 (JSPS) 国際事業委員会書面審査員・書面評価員  
(2014年8月~2016年7月).

Masafumi Shirai, an examiner/evaluator of application, International Exchange Committee,  
Japanese Society for the Promotion of Science (JSPS), (August 2014 - July 2016).

(4) アウトリーチ活動 / Outreach activities

該当なし N/A

4. 競争的資金の獲得状況 / Research funds/grants received

(1) 科学研究費補助金 / Grant-in-Aid for Scientific Research (KAKENHI)

[1]

研究課題：水素化合物の金属化及び超伝導の理論研究

期 間：2013年度~2015年度

研究種目：基盤研究 (C)

研究代表者：阿部和多加

研究経費：総額 4,940,000 円

Research Title: Theoretical study of metallization and superconductivity of hydrides

Research Term: FY2013 - FY2015

Category: Grant-in-Aid for Scientific Research (C)

Principal Investigator: Kazutaka Abe

Research Expenditure: Total 4,940,000 JPY

[2]

研究課題：規則合金スピントロニクス材料の新展開

期 間：2013年度~2017年度

研究種目：基盤研究 (S)

研究代表者：高梨弘毅 (東北大学)

研究分担者：Gerrit E. W. Bauer, 白井正文, 水口将輝, 桜庭裕弥, 関 剛斎

研究経費：総額 9,500,000 円 (分担金)

Research Title: New development of ordered-alloy materials for spintronics

Research Term: FY2013 - FY2017

Category: Grant-in-Aid for Scientific Research (S)  
Principal Investigator: Koki Takanashi (Tohoku Univ.)  
Co-investigators: Gerrit E. W. Bauer, Masafumi Shirai, Masaki Mizuguchi, Yuya Sakuraba, Takeshi Seki  
Research Expenditure: Total 9,500,000 JPY (a share of the expenses)

[3]

研究課題：強誘電体障壁強磁性トンネル接合素子の開発と電界効果によるスピン輸送制御  
期 間：2014 年度～2016 年度  
研究種目：基盤研究（A）  
研究代表者：角田匡清（東北大学）  
研究分担者：末益 崇, 白井正文, 古門聡士, 磯上慎二  
研究経費：総額 1,000,000 円（分担金）  
Research Title: Development of ferromagnetic tunnel-junction devices with ferroelectric barrier and electric-field control of spin transport properties  
Research Term: FY2014 - FY2016  
Category: Grant-in-Aid for Scientific Research (A)  
Principal Investigator: Masakiyo Tsunoda (Tohoku Univ.)  
Co-investigators: Takashi Suemasu, Masafumi Shirai, Satoshi Kokado, Shinji Isogami  
Research Expenditure: Total 1,000,000 JPY (a share of the expenses)

[4]

研究課題：金属人工格子ルネサンス  
期 間：2018 年度～2022 年度  
研究所目：基盤研究（S）  
研究代表者：高梨弘毅（東北大学）  
研究分担者：伊藤啓太, 関 剛斎, 内田健一, 白井正文  
研究経費：1,200,000 円（分担金 2018 年度）  
Research Title: Renaissance of metallic artificial superlattices  
Research Term: FY2018 - FY2022  
Category: Grant-in-Aid for Scientific Research (S)  
Principal Investigator: Koki Takanashi (Tohoku Univ.)  
Co-investigators: Keita Ito, Takeshi Seki, Ken-ichi, Uchida, Masafumi Shirai  
Research Expenditure: 1,200,000 JPY (a share of the expenses in FY2018)

(2) 受託研究費 / Other grants and subsidies

[1]

研究課題：ラティスエンジニアリングによる高磁化磁性材料の創製  
および高性能永久磁石材料の開発  
期 間：2014 年度～2016 年度  
資金制度：科学技術振興機構（JST）産学共創基礎基盤研究プログラム  
「革新的次世代高性能磁石創製の指針構築」  
研究代表者：嶋 敏之（東北学院大学）  
研究分担者：土井正晶, 岡田宏成, 白井正文  
研究経費：総額 2,807,000 円（分担金）  
Research Title: Creation of magnetic materials with high magnetization and development of high-performance permanent magnets by lattice engineering  
Research Term: FY2014 - FY2016  
Funding System: Japan Science and Technology Agency (JST),

Fundamental Research Program for Industry-Academia Co-creation: “Construction of guidelines for creation of innovative, next-generation, and high-performance magnets”  
Principal Investigator: Toshiyuki Shima (Tohoku Gakuin Univ.)  
Co-investigators: Masaaki Doi, Hironari Okada, Masafumi Shirai  
Research Expenditure: 2,807,000 JPY (a share of the expenses)

[2]

研究課題：新概念スピントロニクス素子創製のための国際研究拠点形成  
期 間：2015 年度～2019 年度  
資金制度：日本学術振興会 (JSPS) 研究拠点形成事業 A. 先端拠点形成型  
研究代表者：大野英男 (2015 年度～2017 年度) / 白井正文 (2018 年度～)  
研究経費：総額 72,397,000 円

Research Title: International research center for new-concept spintronics devices  
Research Term: FY2015 - FY2019  
Funding System: Japanese Society for the Promotion of Science (JSPS),  
Core-to-Core Program: A. Advanced Research Networks  
Principal Investigator: Hideo Ohno (FY2015 - FY2017) / Masafumi Shirai (FY2018 - )  
Research Expenditure: Total 72,397,000 JPY

[3]

研究課題：スピントロニクス材料設計  
期 間：2016 年度～2018 年度  
資金制度：総合科学技術・イノベーション会議 (CSTI)  
革新的研究開発推進プログラム (ImPACT)  
「無充電で長期間使用できる究極のエコ IT 機器の実現」  
研究代表者：白井正文  
研究経費：総額 9,100,000 円

Research Title: Spintronics materials design  
Research Term: FY2016 - FY2018  
Funding System: Council for Science, Technology and Innovation (CSTI),  
Impulsing Paradigm Change through Disruptive Technologies Program (ImPACT):  
“Achieving ultimate green IT devices with long usage time without charging”  
Principal Investigator: Masafumi Shirai  
Research Expenditure: Total 9,100,000 JPY

[4]

研究課題：軽元素添加による高磁化磁性材料の創製ならびに革新的永久磁石材料の開発  
期 間：2016 年度～2019 年度  
資金制度：科学技術振興機構 産学共創基礎基盤研究プログラム  
「革新的次世代高性能磁石創製の指針構築」  
研究代表者：嶋 敏之 (東北学院大学)  
研究分担者：土井正晶, 岡田宏成, 白井正文  
研究経費：総額 13,000,000 円 (分担金)

Research Title: Creation of magnetic materials with high magnetization and development of innovative permanent magnets by doping light elements  
Research Term: FY2016 - FY2019  
Funding System: Japan Science and Technology Agency (JST),  
Fundamental Research Program for Industry-Academia Co-creation: “Construction of

guidelines for creation of innovative, next-generation, and high-performance magnets”  
Principal Investigator: Toshiyuki Shima (Tohoku Gakuin Univ.)  
Co-investigators: Masaaki Doi, Hironari Okada, Masafumi Shirai  
Research Expenditure: 13,000,000 JPY (a share of the expenses)

[5]

研究課題：計算科学を用いた磁気抵抗スイッチ素子基盤材料の創出  
期 間：2017年度～2022年度  
資金制度：科学技術振興機構（JST）戦略的創造研究推進事業（CREST）  
「実験と理論・データ科学を融合した材料開発の革新」  
研究代表者：水上成美（東北大学）  
研究分担者：廣畑貴文, 白井正文  
研究経費：総額 70,000,000 円（分担金）

Research Title: Creation of fundamental materials for magnetoresistive switching devices using computational science  
Research Term: FY2017 - FY2022  
Funding System: Japan Science and Technology Agency (JST),  
Strategic Basic Research Program (CREST): “Revolutional material development by fusion of strong experiments with theory/data science”  
Principal Investigator: Shigemi Mizukami (Tohoku Univ.)  
Co-investigators: Atsufumi Hirohata, Masafumi Shirai  
Research Expenditure: 70,000,000 JPY (a share of the expenses)

## 5. 国際共同研究・連携研究・連携教育活動の実績

International joint research, collaborative research, and collaborative education

[1]

研究課題：新概念スピントロニクス素子  
期 間：2015年度～  
共同研究者：Kevin O’Grady（ヨーク大学）  
Burkard Hillebrands（カイザーラウテルン工科大学）  
Research Title: New-concept spintronics devices  
Research Term: FY2015 -  
Co-investigators: Kevin O’Grady (Univ. of York), Burkard Hillebrands (TH Kaiserslautern)

[2]

研究課題：高スピン偏極磁性体を用いたトンネル磁気抵抗素子の理論設計と実証  
期 間：2016年度～  
共同研究者：廣畑貴文（ヨーク大学）  
Research Title: Computational design and realization of tunneling magnetoresistance devices using highly spin-polarized magnets  
Research Term: FY2016 -  
Co-investigators: Atsufumi Hirohata (Univ. of York)

## 6. 共同利用・共同研究拠点活動の実績

Achievements of work done under the framework of Joint Usage/Research Center

[1]

研究課題：強磁性形状記憶合金をはじめとする機能性磁性材料の電子構造と物性発現機構の解明（H25/A04）



期 間 : 2013 年度～2015 年度  
研究代表者 : 今田真 (立命館大学)  
通研対応教員 : 白井正文  
Research Title: Electronic structure and properties of ferromagnetic shape memory and other functional magnetic materials (H25/A04)  
Research Term: FY2013-FY2015  
Principal Investigator: Shin Imada (Ritsumeikan Univ.)  
Collaborator of RIEC: Masafumi Shirai

[2]

研究課題 : 磁性の電界制御の物理と応用 (H25/B04)  
期 間 : 2013 年度～2015 年度  
研究代表者 : 白井正文  
通研対応教員 : 白井正文  
Research Title: Physics and applications of electric-field control of magnetism (H25/B04)  
Research Term: FY2013-FY2015  
Principal Investigator: Masafumi Shirai  
Collaborator of RIEC: Masafumi Shirai

[3]

研究課題 : スピントロニクス学術連携 (H26/S2)  
期 間 : 2014 年度～2016 年度  
研究代表者 : 田中雅明 (東京大学)  
通研対応教員 : 白井正文  
Research Title: Spintronics academic alliance (H26/S2)  
Research Term: FY2014-FY2016  
Principal Investigator: Masaaki Tanaka (Tokyo Univ.)  
Collaborator of RIEC: Masafumi Shirai

[4]

研究課題 : 強誘電体障壁を有する  $\text{Fe}_4\text{N}$  基トンネル接合素子の開発 (H26/A04)  
期 間 : 2014 年度～2016 年度  
研究代表者 : 角田匡清 (東北大学)  
通研対応教員 : 白井正文  
Research Title: Development of  $\text{Fe}_4\text{N}$ -based magnetic tunnel junctions with ferroelectric tunnel barrier (H26/A04)  
Research Term: FY2014-FY2016  
Principal Investigator: Masakiyo Tsunoda (Tohoku Univ.)  
Collaborator of RIEC: Masafumi Shirai

[5]

研究課題 : 磁性体/半導体ハイブリッド構造の形成とナノデバイスへの応用に関する研究 (H26/A05)  
期 間 : 2014 年度～2016 年度  
研究代表者 : 松倉文礼 (東北大学)  
通研対応教員 : 大野英男 (2014 年度) / 白井正文 (2015～2016 年度)  
Research Title: Studies on fabrication of ferromagnet/semiconductor hybrid structures and their application for spintronics devices (H26/A05)  
Research Term: FY2014-FY2016  
Principal Investigator: Fumihiko Matsukura (Tohoku Univ.)  
Collaborator of RIEC: Hideo Ohno (FY2014) / Masafumi Shirai (FY2015-FY2016)

[6]

研究課題：磁性体/半導体ハイブリッド構造の形成とナノデバイスへの応用に関する研究  
(H29/A01)

期 間：2017 年度

研究代表者：松倉文礼（東北大学）

通研対応教員：白井正文

Research Title: Studies on fabrication of ferromagnet/semiconductor hybrid structures and their application for spintronics devices (H29/A01)

Research Term: FY2017

Principal Investigator: Fumihito Matsukura (Tohoku Univ.)

Collaborator of RIEC: Masafumi Shirai

[7]

研究課題：第一原理ナノ構造設計手法の開発（H29/B04）

期 間：2017 年度

研究代表者：下司雅章（大阪大学）

通研対応教員：阿部和多加

Research Title: Development of ab initio methods for nanostructure design (H29/B04)

Research Term: FY2017

Principal Investigator: Masaaki Geshi (Osaka Univ.)

Collaborator of RIEC: Kazutaka Abe

## 7. 研究教育指導 / Research supervision

### (1) 担当講義リスト / List of lectures

[1]

期間：2013年度～2018年度（第1セメスター）

対象：東北大学工学部 1年生

科目：基礎ゼミ（情報社会を支えるデバイスの物理と技術）

担当：辻川雅人, 白井正文

Course: Fundamental Seminar (Physics and technology of devices supporting information-oriented society)

Term: 1st Semester, General Education (FY2013 - FY2018)

Instructor: Masahito Tsujikawa, Masafumi Shirai

[2]

期間：2013年度～2017年度（第2セメスター）

対象：東北大学工学部 1年生

科目：創造工学研修（コンピューターによる物質設計入門）

担当：阿部和多加

Course: Engineering Design (Introduction to computational materials design)

Term: 2nd Semester, General Education (FY2013 - FY2017)

Instructor: Kazutaka Abe

[3]

期間：2018年度（第3クォーター）

対象：東北大学工学部 1年生

科目：物理学B-1

担当：白井正文

Course: Physics B-1

Term: 3rd Quarter, General Education (FY2018)

Instructor: Masafumi Shirai

[4]

期間：2018年度（第4クォーター）

対象：東北大学工学部 1年生

科目：物理学B-2

担当：白井正文

Course: Physics B-2

Term: 4th Quarter, General Education (FY2018)

Instructor: Masafumi Shirai

[5]

期間：2013年度～2018年度（第4セメスター）

対象：東北大学工学部 電気情報工学科 2年生

科目：解析力学

担当：白井正文

Course: Analytical Mechanics

Term: 4th Semester, School of Engineering (FY2013-FY2018)

Instructor: Masafumi Shirai

[6]

期間：2018年度（第4セメスター）

対象：東北大学工学部 電気情報工学科 2年生

科目：電磁気学I

担当：阿部和多加

Course: Electromagnetism I

Term: 4th Semester, School of Engineering (FY2018)

Instructor: Kazutaka Abe

[7]

期間：2013年度～2017年度（第5セメスター）

対象：東北大学工学部 電気情報工学科 3年生

科目：電気・通信・電子・情報工学実験B

担当：阿部和多加

Course: Laboratory B (electric, communication, electronic, and information engineering)

Term: 5th Semester, School of Engineering (FY2013 - FY2017)

Instructor: Kazutaka Abe

[8]

期間：2013年度～2018年度

対象：東北大学大学院工学研究科 電気系3専攻 博士前期課程

科目：熱・統計力学基礎

担当：白井正文

Course: Thermodynamics and Statistical Mechanics

Term: Master's Program, Graduate School of Engineering (FY2013-FY2018)

Instructor: Masafumi Shirai

[9]

期間：2013年度～2018年度

対象：東北大学大学院工学研究科 電気系3専攻 博士後期課程

科目：先端スピニング工学特論

担当：白井正文

Course: Advanced Spintronics Materials and Engineering

Term: Doctor's Program, Graduate School of Engineering (FY2013-FY2018)

Instructor: Masafumi Shirai

(2) 学位取得者リスト

List of bachelor's, master's and doctoral degree students supervised

学 士 / Bachelor

(2014 年 3 月取得)

[1] 森川志門, 「ホイスラー合金を用いた磁気抵抗デバイスに関する理論研究」

Shimon Morikawa, "A theoretical study on magnetoresistance devices using Heusler alloys"

(2015 年 3 月取得)

[2] 隈田 壮, 「強磁性体／強誘電体接合の電子構造と磁気特性に関する理論研究」

So Kumata, "A theoretical study on electronic structure and magnetic properties of ferromagnet / ferroelectric junctions"

[3] 八重樫佳祐, 「金属強磁性の電界制御における基板材料の役割に関する理論研究」

Keisuke Yaegashi, "A theoretical study on the role of substrate materials in electric-field control of metallic ferromagnetism"

(2016 年 3 月取得)

[4] 加藤真人, 「マルテンサイト変態を示す Co 基ホイスラー合金に関する理論研究」

Makoto Kato, "A theoretical study on Co-based Heusler alloys exhibiting martensitic transformation"

[5] 今 諒磨, 「マルテンサイト変態を示すホイスラー合金の熱物性に関する理論研究」

Ryoma Kon, "A theoretical study on thermal properties of Heusler alloys exhibiting martensitic transformation"

[6] 三橋唯澄, 「高磁化・高磁気異方性 Mn 基ホイスラー合金に関する理論研究」

Yuito Mitsuhashi, "A theoretical study on Mn-based Heusler alloys with high magnetization and high magnetic anisotropy"

(2017 年 3 月取得)

[7] 佐藤正樹, 「強磁性金属／絶縁体界面における磁気異方性の非線形電界変調に関する理論研究」

Masaki Sato, "A theoretical study on non-linear electric-field modulation of magnetic anisotropy in ferromagnetic metal / insulator interfaces"

(2018 年 3 月取得)

[8] 林 拓樹, 「高誘電率酸化物障壁磁気トンネル接合に関する理論研究」

Hiroki Hayashi, "A theoretical study on magnetic tunnel junctions with high dielectric-constant oxide barriers"

[9] 岡戸理功, 「極性酸化物／強磁性金属接合における界面磁気異方性に関する理論研究」

Riku Okado, "A theoretical study on interfacial magnetic anisotropy in polar oxide / ferromagnetic metal junctions"

[10] 武藤陽太, 「Mn-Ge 合金の構造安定性と磁性に関する理論研究」

Yotal Muto, "A theoretical study on structural stability and magnetism of Mn-Ge alloys"

(2019 年 3 月取得)

[11] 山吉 諒, 「強磁性／非磁性金属界面におけるスピン軌道トルクと磁気異方性に関する理論研究」

Ryo Yamayoshi, "A theoretical study on spin-orbital torque and magnetic anisotropy in ferromagnet / non-magnetic metal interfaces"

[12] 渡辺康平, 「六方晶系規則合金における異常ホール効果と異常ネルンスト効果に関する理論研究」

Kohei Watanabe, "A theoretical study on anomalous Hall and Nernst effects in hexagonal ordered alloys"

修 士 / Master

(2013 年 9 月取得)

[1] 周 敏燕, 「遷移金属窒化物電極トンネル磁気抵抗素子に関する理論研究」

MinYan Zhou, "A theoretical study on tunneling magnetoresistance devices with transition-metal nitride electrodes"

(2015 年 3 月取得)

[2] 伊東拓也, 「遷移金属規則合金を用いた巨大磁気抵抗素子に関する理論研究」

Takuya Ito, "A theoretical study on giant magnetoresistance devices using transition-metal ordered alloys"

[3] 小野寺昭, 「ハーフホイスラー合金を用いた磁気抵抗素子に関する理論研究」

Akira Onodera, "A theoretical study on magnetoresistance devices using half Heusler alloys"

[4] 狩野 駿, 「磁気構造相変態を起こす Co 基ホイスラー合金に関する理論研究」

Shun Kano, "A theoretical study on Co-based Heusler alloys exhibiting magneto-structural phase transformation"

(2016 年 3 月取得)

[5] 森川志門, 「ホイスラー合金を用いた巨大磁気抵抗素子に関する理論研究」

Shimon Morikawa, "A theoretical study on giant magnetoresistance devices using Heusler alloys"

(2018 年 3 月取得)

[6] 隈田 壮, 「強誘電体障壁磁気トンネル接合における磁性と伝導に及ぼす電気分極の効果に関する理論研究」

So Kumata, "A theoretical study on the effect of electric polarization on magnetic and transport properties in magnetic tunnel junctions with ferroelectric barrier"

[7] 呉 寒, 「高スピン偏極ホイスラー合金／非磁性合金界面における電気伝導に関する理論研究」

Han Wu, "A theoretical study on electric transport at highly spin-polarized Heusler alloy / non-magnetic alloy interfaces"

[8] 今 諒磨, 「Co 基強磁性形状記憶合金の構造相変態に関する理論研究」

Ryoma Kon, "A theoretical study on structural phase transformation in Co-based ferromagnetic shape memory alloys"

[9] 三橋唯澄, 「高磁化・高磁気異方性を有する Mn 基規則合金に関する理論研究」

Yuito Mitsuhashi, "A theoretical study on Mn-based ordered alloys having high magnetization and high magnetic anisotropy"

(2018 年 9 月取得)

[10] 金村卓郎, 「機械学習を用いた四元ホイスラー合金の物性予測に関する研究」

Takuro Kanemura, "A theoretical study on prediction of physical properties of quaternary Heusler alloys by using machine learning"

(2019 年 3 月取得)

[11] 佐々木颯清, 「軽元素添加 FeNi 規則合金における磁気特性および原子拡散過程に関する理論研究」

Ryusei Sasaki, "A theoretical study on magnetic properties and atomic diffusion processes in FeNi ordered alloy doped with light elements"

[12] 佐藤正樹, 「ホイスラー合金/MgO 界面における磁気異方性電圧制御に関する理論研究」

Masaki Sato, "A theoretical study on voltage control of magnetic anisotropy at Heusler alloy/MgO interfaces"

## 8. 叙勲・受賞・表彰 / Honors, awards, and prizes

[1] 白井正文, 平成 27 年度 特別研究員等審査会専門委員 (書面担当) 表彰, 日本学術振興会, (2016 年 7 月 31 日表彰).

Masafumi Shirai, Commendation for expert advisors, Screening Committee of Research Fellowship for Young Scientists, Japanese Society for the Promotion of Science (JSPS), (awarded on 31 July, 2016).

## 9. その他 / Others

該当なし N/A