

# ICC-IMR FY2023 Activity Report

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ICC-IMR FY2023

# Activity Report

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**International Collaboration Center**

Institute for Materials Research  
Tohoku University

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# Mission

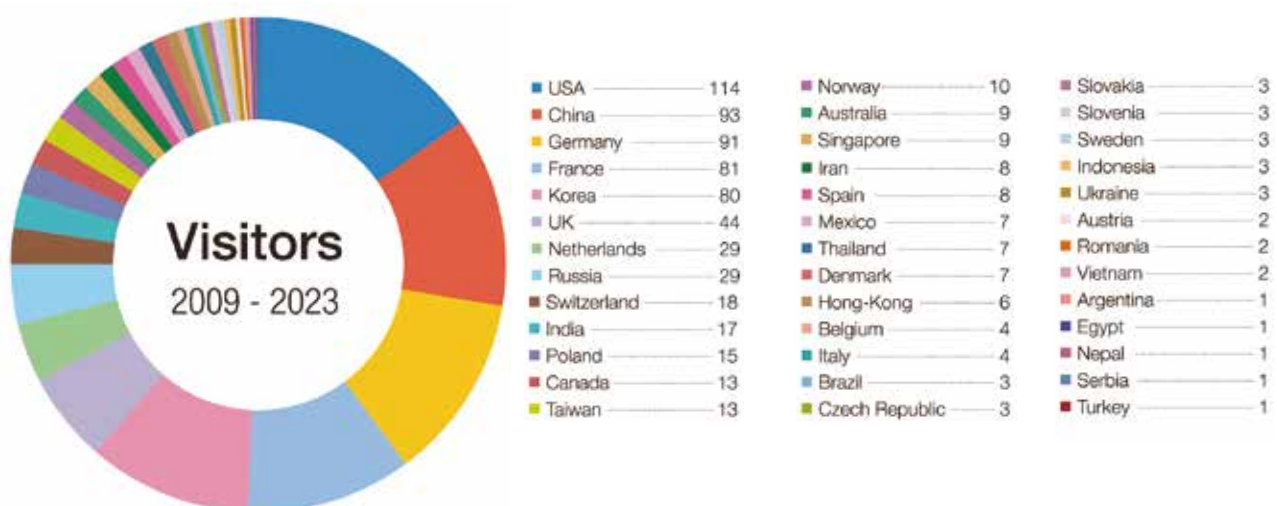
The ICC-IMR was founded in April 2008 as the center for international collaboration of the Institute for Materials Research (IMR) a center of excellence in material science, consisting of 27 research groups and five research centers. The ICC-IMR works as a gateway of diverse collaborations between overseas and IMR researchers. The ICC-IMR has invited 87 visiting professors and conducted 23 international research projects since its start-up (please inspect the graph below for more details,). The applications are open to foreign researchers and the projects are evaluated by a peer-review process involving international reviewers.

ICC-IMR coordinates five different programs:

- 1) International Integrated Project Research
- 2) Visiting Professorships
- 3) International Workshops
- 4) Fellowship for Young Researcher and PhD Student
- 5) Material Transfer Program

We welcome applicants from around the globe to submit proposals!

Visitors supported by ICC-Programs







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Activity Report

Visiting Professors



## Visiting Professors

| No.  | Title in IMR                 | Name                   | Affiliation                                                                                                                 | Host Professor          | Proposed Research                                                                                                            | Term                 |
|------|------------------------------|------------------------|-----------------------------------------------------------------------------------------------------------------------------|-------------------------|------------------------------------------------------------------------------------------------------------------------------|----------------------|
| 22G6 | Visiting Professor           | Junichiro Kono         | Rice University, USA                                                                                                        | Prof. Nojiri            | Spectroscopy of Matter in High Magnetic Fields                                                                               | 2022.10.1-2023.9.30  |
| 22G9 | Visiting Associate Professor | Anna Kosogor           | Institute of Magnetism of National Academy of Sciences of Ukraine and Ministry of Education and Science of Ukraine, Ukraine | Prof. Umetsu            | Influence of the Chemical Composition on the Magnetocaloric Properties of Metamagnetic Shape Memory Alloys                   | 2023.5.10-2023.10.31 |
| 23G1 | Visiting Professor           | Jun-Sik Lee            | SLAC National Accelerator Laboratory, USA                                                                                   | Prof. Nojiri            | Developing Resonant Soft X-ray Scattering Technique in Very High Magnetic Fields by Using Advanced Pulse Magnet Design       | 2023.6.21-2023.7.20  |
| 23G2 | Visiting Professor           | Michael Zhitomirsky    | Interdisciplinary Research Institute of Grenoble (IRIG), CEA, France                                                        | Prof. Nojiri            | Phase Diagrams and Competing Interactions in Complex Triangular Antiferromagnets                                             | 2023.10.1-2023.11.30 |
| 23G3 | Visiting Lecturer            | Mohammad Saeed Bahramy | University of Manchester, UK                                                                                                | Assoc. Prof. Belosludov | Modelling Emergent Quantum Phases in Two-Dimensional Materials                                                               | 2023.6.16-2023.8.7   |
| 23G4 | Visiting Professor           | Ilya Sheikin           | LNCMI, CNRS, France                                                                                                         | Prof. Aoki              | Electronic Structure and Fermi Surfaces of Ce-Based Heavy-Fermion Compounds                                                  | 2023.7.1-2023.9.30   |
| 23G5 | Visiting Associate Professor | Toni Helm              | The Helmholtz Zentrum Dresden Rossendorf (HZDR), Germany                                                                    | Assoc. Prof. Kimata     | Angle-Dependent Magnetoresistance Studies in the Spin-Triplet Superconductor UTe <sub>2</sub>                                | 2023.4.1-2024.3.31   |
| 23G6 | Visiting Professor           | Daniel Braithwaite     | CEA Grenoble, France                                                                                                        | Prof. Aoki              | Calorimetry in Miniature Diamond Anvil Cell                                                                                  | 2023.11.6-2023.12.18 |
| 23G7 | Visiting Associate Professor | Ilya Okulov            | Leibniz-Institut für Werkstofforientierte Technologien (IWT), Germany                                                       | Prof. Kato              | Design of Integrated Composite Electrode Composed of Porous Metallic Current Collector and Nanoscale Active Ceramic Material | 2024.3.1-2024.3.29   |
| 23G8 | Visiting Assistant Professor | Soo-Hyun Joo           | Dankook University, Korea                                                                                                   | Prof. Kato              | Dissimilar Bonding via 3D Interconnected Structures of Liquid Metal Dealloying                                               | 2024.1.30-2024.2.27  |

## Spectroscopy of Matter in High Magnetic Fields

We report on near-infrared and visible spectroscopy in high magnetic fields. The acquisition of the 50 T pulsed magnet combined with the IR-VIS spectroscopy system has been improved from one data point per magnetic pulse shot to twelve data points in a single magnet pulse shot. The g-factor and the diamagnetic shift have been measured in two-dimensional Ruddlesden-Popper perovskites.

The two-dimensional (2D) Ruddlesden-Popper (RP) perovskites form quantum wells by sandwiching inorganic-organic perovskite layers used in photovoltaic devices between organic layers [1]. The perovskite layer thickness defined by the integer value  $n$  in  $(\text{BA})_2(\text{MA})_{n-1}\text{Pb}_n\text{I}_{3n+1}$  determines their optical properties. Here, investigated samples with  $n=5$  using IR-VIS magnetospectroscopy up to 40 T.

The 50 T-capable RAMBO-II IR/VIS magnet produces a nearly 2 ms duration asymmetric magnetic field pulse (see Fig. 1) at intervals of 57 seconds for every Tesla above 7 Tesla at the peak. The scale of access to this magnet compared to the limited time available at national facilities is an incredible boon and enables us to specialize the surrounding experiment to be even more efficient in data collection. Our experimental system can measure magneto-optical properties at 14 distinct times in 12 different fields during a single pulse. An entire field sweep can thus be accomplished with a single button press. Due to the increasing resistance from Joule heating, the asymmetric pulse shape gives slower rates of change in magnetic field and increases the time available to sample more fields with less variation.

Figure 1a) shows the magnetic pulse profile in blue. Laser pulses are in red, and camera exposure intervals are in orange. The data can be acquired by the CCD camera (see images in Fig. 1b)) for each laser pulse shown Fig. 1a). The inset in Fig. 1 shows the distribution of magnetic fields that can currently be sampled from one 40 T pulse. The pulse shape does not scale linearly, but the distribution at 50T is expected to be comparable. In this way, all the magneto-optical data for material across the full -50 to +50T range,  $\sigma^+$  and  $\sigma^-$  (circularly polarized light), at a given temperature can be taken with only four pulses of the magnet. The final incremental upgrade to 50 T is also expected to coincide with additional experimental improvements, increasing the acquisition rate of spectroscopic data and, thus, the total number and density of sampled fields.

The 50T IR/VIS system is first applied to studying 2D RP perovskites. In these hybrid solar cell materials, layers of methylammonium lead iodide are stacked between insulating layers of

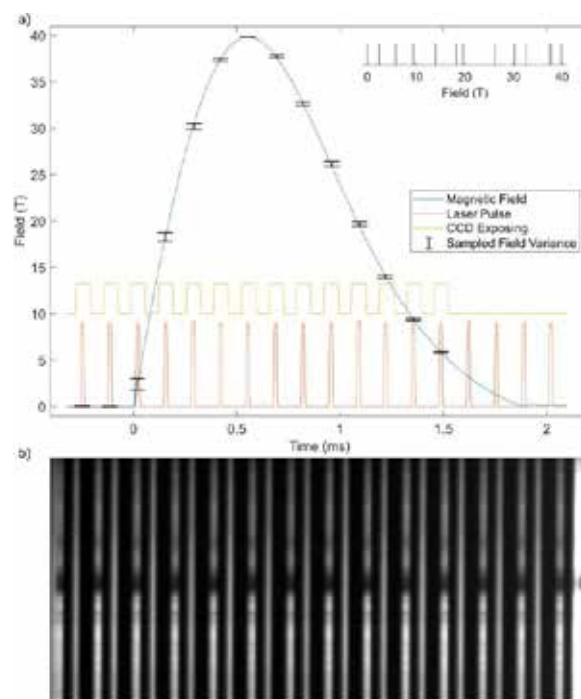


Fig. 1. a) Magnetic pulse profile (blue) together with light pulse train (red) and exposure intervals (orange). Black dots with error bars show magnetic fields for which data can be acquired for a single magnetic pulse shot. The inset shows the distribution of fields that can be sampled from a single magnetic pulse with the 40T peak field. b) Each image is a frame taken by the camera, corresponding to a sampling of the magnetic field in the a) plot.

butylammonium to create a pseudo-quantum-well structure. The inclusion of butylammonium provides additional chemical stability to the famously reactive perovskite, but the 2D confinement enhances the exciton interaction – increasing their binding energy and reducing the rate of free carrier escape under photoexcitation.

The studies of the diamagnetic shift via magnetospectroscopy grant insight into the changing size of the exciton at different temperatures, which we are using as part of a paper-in-preparation to make some predictions about the much harder-to-measure exciton binding energy in these materials. This experimental setup has allowed us to experiment with a broad set of permutations on material parameters, namely stacking order, orientation,

and temperature. The number of measurements this growing parameter space requires becomes prohibitive when experiment time is limited at a high magnetic field facility but can be accommodated with in-house experiments.

Figure 2a) shows an image mounted into a 50 T magnet. The sample is situated on the sapphire pipe connected to the sample cryostat. The transmitted light is collected using the fiber located right below the sample. We have conducted transmission experiments for both right and left circularly polarized light in the -40 T and +40 T magnetic field ranges. Figure 2b) shows exemplary data for the exciton attenuated of 2D RP perovskite  $n=5$ , at 0, +40 T for right and left circularly polarized light. As one can see, the exciton peaks shift in opposite directions based on light chirality, but this shift is asymmetric due to a larger contribution of diamagnetic shift.

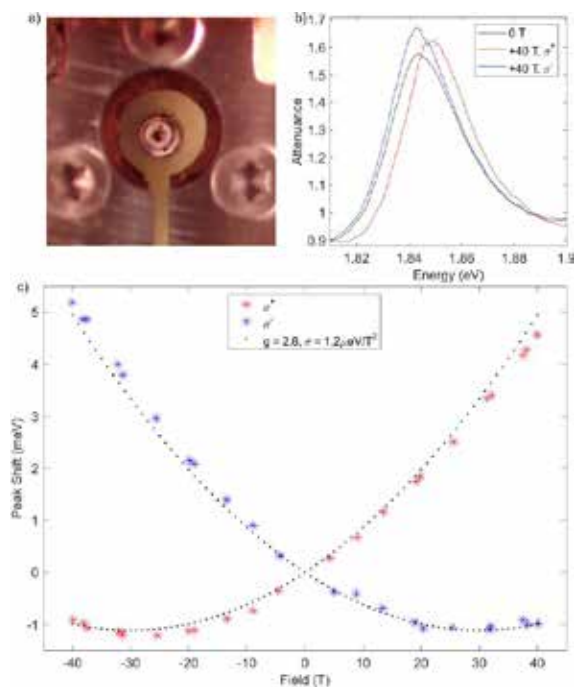


Fig. 2. a) an optical image of a 50T coil with the mounted sample. b) Attenuance spectra of  $(\text{BA})_2(\text{MA})_{n-1}\text{Pb}_n\text{I}_{3n+1}$  for  $n=5$  at 0 T and 40 T for two circular polarizations. c) Exciton peak shift as a function of magnetic field for two circular polarizations. The dashed line is the fit.

Figure 2c) summarizes exciton peak shift as a function of the magnetic field at different light polarizations. The data was fitted to the equation [2]:

$$E = E(B = 0) \pm \frac{1}{2}g\mu_B B + \sigma_0 B^2,$$

resulting in  $g = 2.7$  and  $\sigma = 1.6 \mu\text{eV/T}^2$ .

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Keywords: exciton, optical properties

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## Influence of Chemical Composition on the Functional Properties of $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$ Metamagnetic Shape Memory Alloys

Sb addition to AFM  $\text{Ni}_{50}\text{Mn}_{50}$  alloy induces FM interaction and lowers Néel temperature. Dependence of Néel temperature on Sb content was computed for  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  alloys. Temperature-composition phase diagram of  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  system was constructed. Competing AFM and FM interactions lead to a spin glass state. Magnetic ordering significantly affects low-temperature specific heat and electronic coefficient.

Ni-Mn-based magnetic shape memory alloys possess distinctive properties such as the magnetocaloric effect, elastocaloric effect, shape memory effect, superelasticity, and giant magnetoresistance, making them highly promising for various applications. Among these, the Ni-Mn-Z ( $Z = \text{In}, \text{Sn}, \text{Sb}$ ) system is notable for its rich phase diagram and the possibility to tailor its functional properties through alloying with Z elements. In particular, in  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Z}_x$  alloys, the martensitic transformation (MT) occurs at lower Z concentrations, whereas higher Z concentrations keep the alloy in a parent ferromagnetic (FM) austenitic phase. The low-temperature martensitic phase of  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Z}_x$  alloys remains a topic of ongoing research.

In this work, we have conducted a comprehensive study on  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  alloys [2]. Through a combination of magnetization experiments, differential scanning calorimetry, low-temperature specific heat measurements, along with its theoretical analysis, we have elucidated the intricate magnetic and electronic properties of this alloy system. Our primary objective has been to unravel the fundamental aspects of magnetic transitions within the Ni-Mn-Sb alloy system. Additionally, we have constructed a temperature-concentration phase diagram for Ni-Mn-Sb alloys, thereby contributing to a more thorough understanding of its phase behavior.

The altering Sb content in  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  alloys induces variations in magnetic interactions and phase transitions. The addition of Sb to  $\text{Ni}_{50}\text{Mn}_{50}$ , which is collinear antiferromagnet (AFM) with a high Néel temperature, induces ferromagnetic interaction and leads to the decrease of Néel temperature. The compositional dependence of Néel temperature was computed from magnetic data. Increasing Sb content reduces characteristic temperatures for AFM interaction and elevates characteristic temperatures for FM interaction. Fig. 1 displays the characteristic

temperature of AFM (blue region) and FM (red region) interaction in  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  system. The overlap of these regions gives rise to a spin glass state [2]. The blue line corresponds to MT transition temperature. We identified six distinct magnetic phases in the  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  system depending on temperature and Sb concentration as shown in Fig. 1. It includes: antiferromagnetic martensite (AFM M), paramagnetic martensite (PM M), ferromagnetic martensite (FM M), spin glass or blocking state (SG or BS) within the martensitic state, and paramagnetic austenite (PM A) and ferromagnetic austenite (FM A) within the austenitic state.

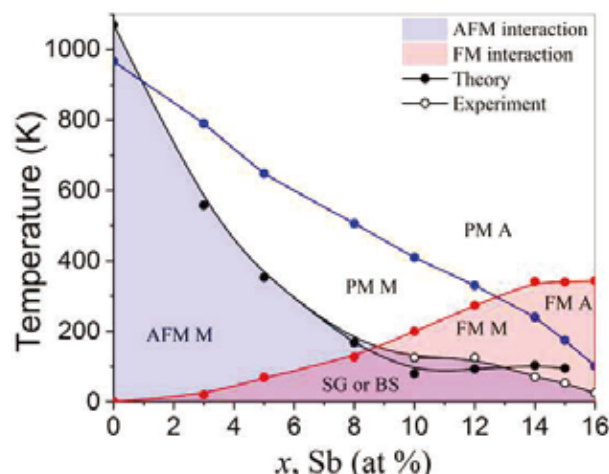


Fig. 1 The AFM (blue region) and FM (red region) interactions in  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  system giving rise to spin glass state (pink region). Characteristic temperatures of AFM interaction: computed (black circles) and estimated from experiments (open circles).

The experimental investigation of low-temperature specific heat of metallic alloys is of considerable significance due to its close connection to the underlying electronic properties. Indeed, the analysis of measurements of low-temperature specific heat is commonly used for the empirical estimation of electronic specific heat

coefficient  $\gamma$  and Debye temperature  $T_D$ . However, in the case of consideration of magnetic solid the influence of the magnetic ordering should be accurately accounted for the proper estimation of the electronic, lattice, and magnetic contributions to the specific heat [3]. Understanding specific heat behavior in relation to magnetic ordering is crucial for characterizing the thermodynamic and electronic properties of magnetic materials. This influence is especially pronounced for metamagnetic Ni-Mn-Z ( $Z = \text{In, Sn, Sb}$ ) alloys, where the drastic changes in the magnetic characteristics occur depending on  $Z$  concentration.

In present work it has been shown that low-temperature specific heat measured for  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  alloys with  $x \geq 17$  being in the FM parent state is significantly different from that measured for the alloys, with  $x \leq 16$ , being in martensitic phase with weak magnetism. Through a detailed experimental analysis and theoretical considerations, we aim to accurately estimate the electronic, magnetic and lattice contributions to low-temperature specific heat and explore the dependence of the  $\gamma$  and  $T_D$  on Sb content in both parent and martensite phases [2].

The procedure for the evaluation of the magnetic part of the specific heat of FM solid was elaborated in [3]. The application of this procedure to different  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  alloys resulted in the concentration dependence of electronic specific heat coefficient and Debye temperature shown in Fig. 2. For the FM austenite region, the filled circles represent the electronic specific heat coefficient and Debye temperature calculated with the account of the magnetic contribution to specific heat (non-linear fit), while open circles denote results from the linear fit, which excludes the magnetic system's contribution. It is seen that disregard of the magnetic contribution in this phase results in an overestimation of the electronic coefficient by a factor of 2 and noticeable underestimation of the Debye temperature.

Importantly, the described behavior may extend to other  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Z}_x$  ( $Z = \text{In, Sn}$ ) alloys, where the addition of  $Z$  elements leads to the introduction of ferromagnetic interaction.

The results of this collaborative study were published in [2], and support from ICC-IMR was acknowledged.

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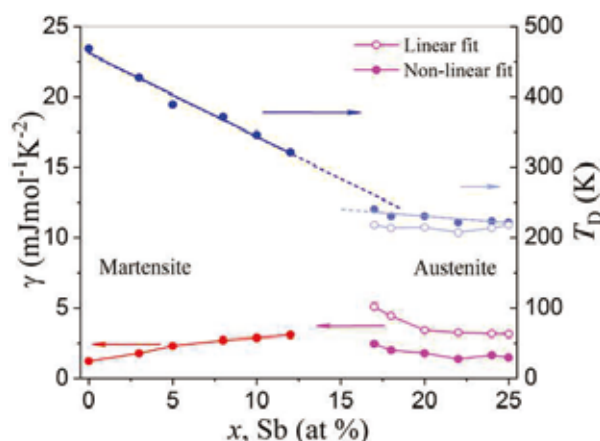


Fig. 2 Evaluated electronic specific heat coefficient  $\gamma$  and Debye temperature  $T_D$  of  $\text{Ni}_{50}\text{Mn}_{50-x}\text{Sb}_x$  alloys as a function of concentration  $x$ . The filled circles show  $\gamma$  and  $T_D$  estimated with the account of magnetic contribution to the specific heat (non-linear fit), while the open circles correspond to the linear fit, which disregards the contribution of magnetic system. Lines are guides for eyes.

Keywords: magnetic properties, specific heat, phase transformation  
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## Title: Developing resonant soft x-ray scattering technique in very high magnetic fields by using advanced pulse magnet design

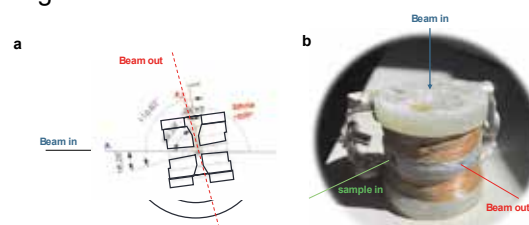
**Introductory part: (Abstract)** The IMR team's extensive efforts have established the well-established use of X-ray techniques with a pulsed field magnet to explore complex phenomena in quantum materials. Here, we proposed moving one step further and developing a pulsed magnet with resonant soft X-ray scattering, enhancing our understanding of correlated electrons, particularly in high-temperature superconductors, under unprecedented magnetic fields.

Combining x-ray techniques with a magnetic field provides a groundbreaking set of advanced probes for quantum materials. This approach offers unique opportunities to unveil profound scientific phenomena, such as complex and exotic states in strongly correlated electron systems. When an applied magnetic field ( $H$ ) reaches approximately 50 Tesla, its corresponding Zeeman energy ( $\sim 70$  K) approaches the perturbation of the phonon effect. This field strength aligns well with the energy scales of several phenomena observed in high-temperature superconductivity (HTSC) and other quantum materials. Despite this potential, conducting X-ray scattering experiments at fields greater than  $H = 20$  Tesla presents significant technical challenges due to limitations in conventional superconducting DC magnets. Furthermore, x-ray spectroscopy under moderate magnetic fields to investigate correlated electron phenomena in quantum materials remains a highly desired but unachieved goal.

**Proposed Development:** I proposed developing a pulsed magnet to achieve state-of-the-art X-ray instrumentation at SLAC with both macroscopic and microscopic sensitivities for investigating quantum materials. A team at the Institute for Materials Research (IMR) at Tohoku University, led by Professor Nojiri, is uniquely positioned to implement this development. The critical innovation involves integrating a 30 Tesla, ultimately 50 Tesla, pulse magnet with a resonant soft x-ray scattering (RSXS) setup. This development will enable the exploration of correlated electrons and corresponding bonding phenomena in high- $T_c$  superconductors, such as intertwined self-organization forms, for example, charge-density wave (CDW) or its stripe-order, under unprecedented magnetic field strengths.

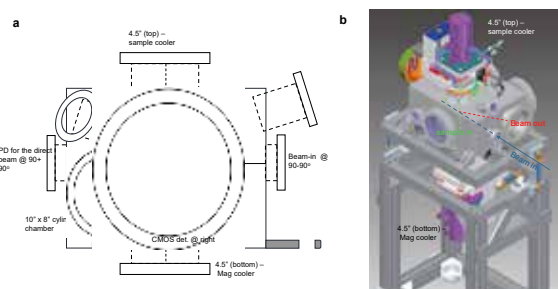
**Project Plan:** I outlined a one-month project for this magnet development at IMR/Tohoku. During my visit, we, together with the Nojiri team, focused on designing and engineering a prototype of the pulsed magnet for RSXS (see Figure 1). Since the soft x-ray has a short wavelength, it was critical to define the scattering

geometry properly. In this sense, we adopted the concept of the split-pair type magnet. Also, the magnet will be rotated with the sample through a different rotation stage to maintain proper open angles.



**Fig. 1: a.** Designed split-pair magnet for RSXS. **b.** The initial prototype magnet was made by the Nojiri team.\_

Upon returning to the home institute at SLAC, I started to design other setups for integrating the magnet into the x-ray setup (Figure 2). Meanwhile, prof. Nojiri and I used the developed RSXS instrumentation for HTSC case studies. As a demonstration, we will initially explore the self-organization forms of paired 3d-electrons in copper-oxide compounds (Y-based cuprate) using RSXS under 30 Tesla. The expected test



**Fig. 2: a.** Schematic drawing for integrating the magnet inside a scattering chamber. **b.** The designed RSXS setup.

run will be by the end of 2024.

**Significance and Impact:** The discovery and utilization of functional materials are vital to our technology-rich society. Materials with strongly correlated electronic systems have the potential to offer new functionalities and pathways to applications. For instance, research on quantum materials paves the way for functional quantum



computers, resistance-free electricity, and many other potentially transformative applications. Unique system-level behavior and related functional properties generally emerge from the intercoupling behavior among constituents such as spin, orbital, charge, and lattice. Our team ultimately discovered a remarkable 3D arrangement of a material's electrons closely linked to the phenomenon of high-temperature superconductivity [1-3].

While investigating the role of CDW in HTSC in the past [1-10], I encountered a limitation related to the sample environment. This is because not only is the magnetic field strength low, but also the spectroscopic information is lacking. Despite our previous efforts [1-3, 9, 10], most of the high magnetic field scattering experiments have been performed at a hard x-ray range, particularly the non-resonant x-ray scattering regimes. Through this proposed development, indeed, we believe that we could overcome the limitation. In particular, the resonant process will shed new light on microscopic information on the field-induced phenomena in high- $T_c$  cuprates, such as the 3D CDW order [1-3].

**Conclusion:** Given my experience, including the Nojiri team's expertise, I believe the proposed development and its successful demonstration can reveal new quantum phases of matter, potentially altering our understanding of the essential physics regarding the mother state in HTSC. Furthermore, the success of this project could reshape our understanding of quantum materials and pave the way for transformative technological applications.

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Keywords: high magnetic field, superconducting, x-ray diffraction (xrd)  
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## Theory of the orthogonal magnetic structure in GdB<sub>4</sub>

Geometrical magnetic frustration combined with competing anisotropies leads to a rich and complex behavior of rare-earth tetraborides RB<sub>4</sub>. In our study we focus on GdB<sub>4</sub>, which exhibits a chiral spin cross antiferromagnetic state in zero magnetic field. We develop a microscopic spin model that explains the origin of this unusual 90° magnetic structure and study the magnetization process in high magnetic fields.

Metallic rare-earth tetraborides exhibit interesting magnetic and electrical properties. Their crystal lattice can be viewed as an array of two-dimensional layers of orthogonal dimers formed by pairs of nearest-neighbor magnetic rare earths, see Fig. 1. This lattice is topologically equivalent to the famous Shastry-Sutherland lattice, which in the case of small spins  $S = 1/2$  and antiferromagnetic interactions hosts an exact spin-liquid state [1]. Rare-earth tetraborides provide an experimental realization of the Shastry-Sutherland model with large spins. GdB<sub>4</sub> is a special member of the tetraboride family, which possess a unique 90° spin structure in zero magnetic field shown in Figure 1 [2]. The origin of such a chiral antiferromagnetic structure as well as the behavior in high magnetic fields [3] remain unexplained to date. In our recent study [4] supported by ICC-IMR, Tohoku University, we address these fundamental questions related to GdB<sub>4</sub> and other planar tetraborides like TbB<sub>4</sub>.

Gadolinium 4f<sup>7</sup> ions have the electronic configuration and are described by the spin-only magnetic moments with  $S = 7/2$ . The minimal spin model for GdB<sub>4</sub> must include at least two exchange constants  $J_1$  and  $J_2$  corresponding to interactions inside and between dimer pairs, see Fig. 1. In the tetragonal crystal lattice of tetraborides, the local symmetry on rare-earth sites is only orthorhombic. Accordingly, the lowest-order crystal-field Hamiltonian has a biaxial form:

$$\hat{\mathcal{H}} = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) + \sum_i [D S_i^z + E(S_i^x - S_i^y)] \quad (1)$$

In addition to the exchange and the single-ion terms  $D$  the above spin Hamiltonian includes the antisymmetric Dzyaloshinskii-Moriya (DM) interactions, which is responsible for a specific chirality in the spin cross state. The DM interactions are forbidden on the dimer bonds because of the inversion symmetry with respect to the bond center. Such symmetry is not present on the second neighbor bonds. Furthermore, because the  $ab$  plane is the mirror plane, the DM vectors on the second-neighbor bonds must be parallel to the  $z$  axis. The corresponding sign convention for the antisymmetric couplings is indicated by arrows on the second neighbor bonds (Fig.1).

We have used the spin Hamiltonian (1) to compute the basic properties of GdB<sub>4</sub>. The observed 90° spin structure is stabilized by a negative in-plane anisotropy constant  $E < 0$ . The chiral state is favored by the positive DM constant  $D_2 > 0$ . Values of the microscopic parameters  $J_1, J_2$  and  $D$  are constrained by the Curie-Weiss temperature  $\theta = -67$  K in GdB<sub>4</sub> and the measured values of the saturation field  $H_s = 52$  T for  $H \parallel [100]$  and 54T for  $H \parallel [001]$  [3]. This procedure gives  $J_1 = 8$ K,  $J_2 = 0.9$ K,  $D = 0.45$ K,  $E = 0.1$ K. We further theoretically simulated the magnetization process in GdB<sub>4</sub> by performing energy minimization on finite lattice clusters starting with random spin configurations. The calculated  $M(H)$  curves are presented in the middle and the right panels of Figure 1.

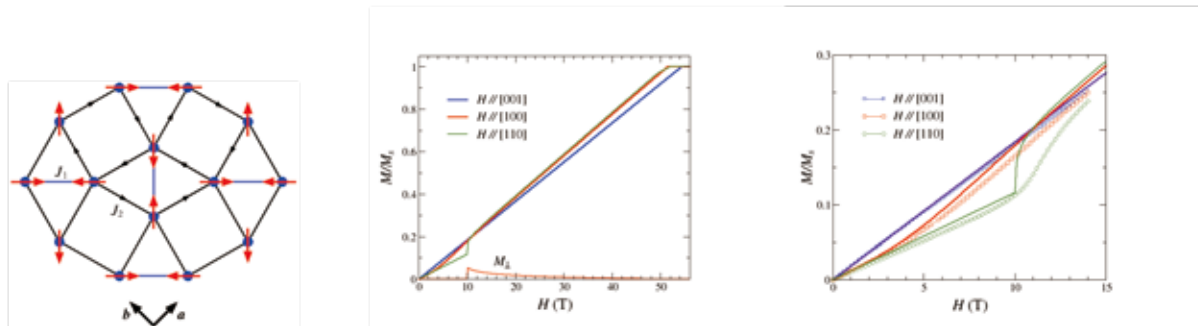


Fig. 1. Left panel: Lattice of gadolinium atoms in GdB<sub>4</sub>. Red arrows show the ordered magnetic moments as observed in the neutron diffraction experiments [2]. Middle panel: Magnetization curves  $M(H)$  computed for the spin model (1) of GdB<sub>4</sub> with  $J_1 = 8$ K,  $J_2 = 0.9$ K,  $D = 0.45$ K,  $E = -0.1$ K for different orientations of an applied field. For  $H \parallel [100]$  the magnetization develops a transverse component above the spin-flop transition at 10T. Right panel: Comparison of the theoretical results to the experimental data [3].

Using our spin model we were able to successfully describe the magnetization process in  $\text{GdB}_4$  for all three principal orientations of the field. Furthermore, we explain an unusual feature on the curve  $H // [110]$  as the spin-flop transition, which affects only a half of Gd spins. The Monte Carlo simulations of the spin model (1) are under way and will further help to validate our set of microscopic parameters by comparing to the observed transition temperature in zero magnetic field.

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## Magnetically Controllable Two-Dimensional Spin Transport in a 3D Crystal

Two-dimensional quantum materials have become a new paradigm in condensed matter physics, offering exciting device applications. Stabilizing and controlling these phases, however, has proven challenging. Here, we propose an innovative method to realize an externally controllable quasi-two-dimensional electronic state with topologically non-trivial spin textures in a three-dimensional perovskite. We further explore their potential implementations in various spintronic applications.

Over the past few years, my group at the University of Manchester has closely collaborated with Professor Rodion Belosludov's team at IMR on several projects focused on modeling emergent quantum phenomena in two-dimensional (2D) materials [1-3]. This collaboration has leveraged the state-of-the-art computational facilities at IMR's Center for Computational Materials Research (CCMS). My visit during the summer of 2023 provided an exceptional opportunity to solidify our joint research on a specific group of Perovskite compounds, establishing them as ideal spintronic candidates for 2D spin transport with novel topological properties [4].

During this visit, our research focused on  $\text{Eu}_{0.5}\text{TaO}_3$ , a prototypical system related to conventional  $\text{ABO}_3$  perovskites such as  $\text{SrTiO}_3$  and  $\text{KTaO}_3$ . In  $\text{Eu}_{0.5}\text{TaO}_3$ , however, the A site is half-filled by the magnetic rare-earth element Eu. As a result, the primitive cell of  $\text{Eu}_{0.5}\text{TaO}_3$  consists of two distorted  $\text{TaO}_3$  octahedra sandwiching a Eu layer, stacked alternately along the crystalline c-axis. This

structure leads to the system being dubbed a *fractional double perovskite* [4].

A key feature of  $\text{Eu}_{0.5}\text{TaO}_3$  is its strong atomic spin-orbit interaction from Ta ions. When combined with the local inversion asymmetry of their  $\text{TaO}_3$  octahedra, this interaction creates two spatially separated Rashba fields with opposite chiralities, as shown in Figure 1. Additionally, the large local Eu 4f-orbital magnetic moments facilitate a delicate yet profound magnetic exchange coupling with the Ta charge carriers through a proximity-induced mechanism known as the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction. Our first-principles calculations revealed [4] that by controlling the interplay between the intrinsic Rashba fields experienced by the charge carriers and the RKKY exchange coupling they mediate among the local Eu magnetic moments through an external magnetic field, they can form quasi-2D energy pockets with topologically non-trivial characteristics, manifested as alternating monopole-anti-monopole-like spin textures, as shown in Fig. 1.

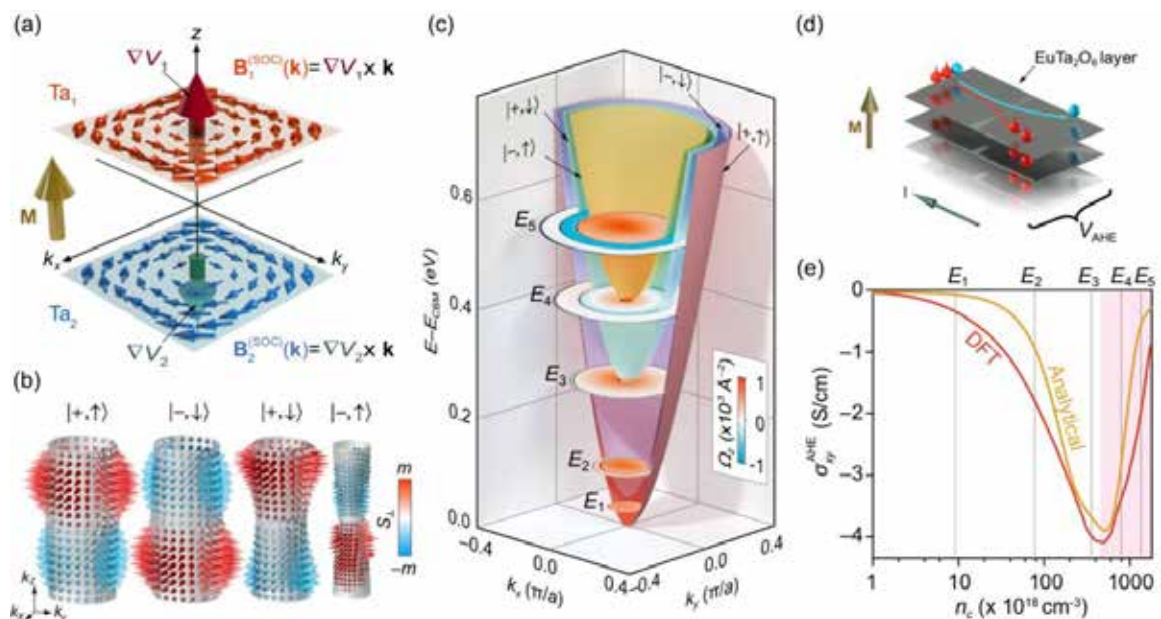


Fig 1. (a) Rashba fields and (b) monopole-anti-monopole-like spin textures in  $\text{Eu}_{0.5}\text{TaO}_3$  conduction bands. The Berry-curvature-projected low-energy electronic structure of  $\text{Eu}_{0.5}\text{TaO}_3$  (c), forming quasi-2D electron gases (d). The resulting Anomalous Hall conductivity is shown in (e).

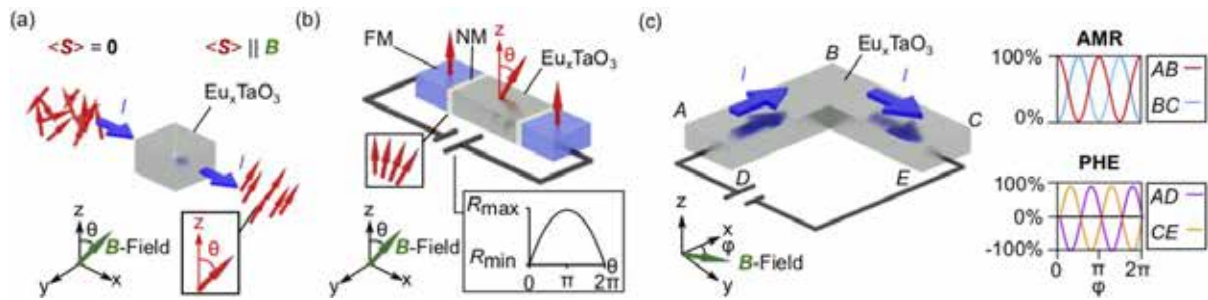


Fig. 2. Spintronic device applications for  $\text{Eu}_x\text{TaO}_3$ . (a) Spin polarizer, generic non-spin polarized current enters material and is spin-polarized along the applied magnetic field  $B$ . (b) Inter-facial spin valve,  $\text{Eu}_x\text{TaO}_3$  has itinerant ferromagnetic (FM) contacts at either end, with a thin non-magnetic (NM) layer separating them. As transport across the FM-NM- $\text{Eu}_x\text{TaO}_3$  junction leads to spin scattering, as shown in the inset, adjusting the polar angle of  $B$ , and thus adjusting the relative angle between the magnetizations, manipulates the resistance across the device. (c) Spin transistor, current flows around the device from A to C under the influence of an angularly variable  $B$ .

Focusing on transport phenomena, we demonstrated that this quasi-2D behavior leads to various anomalies in charge conductivity, including divergent quantum oscillations and an oscillating Seebeck effect. Both effects were proposed as possible probes to observe the interplay experimentally. Furthermore, our calculations suggest that this system and similar materials could exhibit an intrinsic Anomalous Hall Effect (AHE) with a non-monotonic dependence on the charge carrier, offering the possibility of a tunable AHE [4]; See Fig. 1. The origin of this AHE is not fully explained and remains a key area of our ongoing research collaboration.

The remarkable level of controllability over the fermiology and magnetic properties of  $\text{Eu}_{0.5}\text{TaO}_3$  makes this system an ideal candidate for realizing quasi-2D electron gases, applicable in cutting-edge spintronic devices. Inspired by these findings, we proposed several device applications incorporating  $\text{Eu}_{0.5}\text{TaO}_3$ , such as spin polarizers, spin transistors, and interfacial spin valves [4], as shown in Fig. 2.

Building on these findings, we are currently investigating the topological properties of fractional perovskites in more detail and searching for similar materials exhibiting such quantum properties. Through our collaboration with colleagues at IMR, we are confident that our findings can pave the way for establishing a new platform for spintronics with advanced device

functionalities suitable for future energy and quantum information technologies.

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## Fermi Surfaces Detected by de Haas-van Alphen Experiments in $U_2RhIn_8$

We succeeded in growing high quality single crystals of the heavy fermion antiferromagnet  $U_2RhIn_8$  and performed the de Haas-van Alphen (dHvA) experiments. The angular dependence of dHvA frequencies reveals quasi-two dimensional Fermi surfaces as well as small Fermi surfaces. The effective masses are in the range from 2 to  $14m_0$  for the field along c-axis. The experimental results are compared with the LDA band structure calculations associated with both paramagnetic and antiferromagnetic Brillouin zone.

Uranium based heavy fermion compounds exhibit a variety of ground states including the coexistence of ferromagnetism and superconductivity ( $URhGe$ ,  $UCoGe$ ,  $UGe_2$ ), hidden order ( $URu_2Si_2$ ) and more recently a new spin-triplet superconductor  $UTe_2$ . The electronic structures, in particular Fermi surface dimensionality, is a key ingredient to understand such unusual physical properties[1].

In Ce-based heavy fermion superconductors, a prototype is so-called Ce115 and Ce218 systems, which form  $CeTIn_5$  (T: transition metal) and  $Ce_2TIn_8$ , respectively. The structure of  $CeTIn_5$  consists of  $CeIn_3$  and  $TIn_2$  layers, and thus the quasi-two dimensional Fermi surfaces are expected. Indeed, the dHvA experiments revealed the quasi-two-dimensional Fermi surfaces with heavy effective masses in  $CeCoIn_5$  and  $CeIrIn_5$ , which agree well with the results band structure calculations based on the 4f-

itinerant model. In the antiferromagnet  $CeRhIn_5$ , the Fermi surfaces consist of the quasi-two dimensional Fermi surfaces as well, which are explained by the band calculations based on the 4f-localized model. The 4f-itinerant and -localized Fermi surfaces are an important issue from the theoretical point of view related to the “large” and “small” Fermi surfaces.

In  $Ce_2TIn_8$ , the crystal structure can be considered as the stacking of two layers of  $CeIn_3$  and  $TIn_2$ . The degrees of two dimensionality is less than that in  $CeTIn_5$ , as it is confirmed by the dHvA experiments[2,3,4].

$U_2RhIn_8$  crystalizes into a tetragonal crystal structure with space group  $P4/mmm$  (#123). It undergoes an antiferromagnetic transition at a Neel temperature  $T_N = 117$  K. The Sommerfeld coefficient  $\gamma = 47$  mJ K<sup>-2</sup> mol<sup>-1</sup> is rather large given the high Neel temperature. The magnetic structure determined by single-crystal neutron diffraction is commensurate with propagation vector  $Q = (1/2, 1/2, 0)$  and magnetic moments aligned along the c axis.

In order to clarify the electronic structure of  $U_2RhIn_8$  through the dHvA experiments, first we grew high quality single crystals using the In self-flux method. The resistivity and specific heat measurements clearly show the antiferromagnetic transition at  $T_N=117$ K without contaminations of  $UIn_3$  and  $URhIn_5$  as impurity phases. The high quality was demonstrated by the large residual resistivity ratio (RRR=700).

A plate-shaped single crystal was placed in a pickup coil to perform the dHvA experiments with the field-modulation technique. The dHvA experiments were done using a top-loading dilution fridge at low temperature down to 60mK and at high fields up to 15T.

Figure 1(a) shows the typical dHvA oscillations for the field along c-axis. The oscillations are already visible at low field, 6T, indicating the high quality of our sample. The corresponding FFT spectrum is shown in Fig.1(b). One can see fundamental dHvA branches named  $\eta$ ,  $\epsilon$ ,  $\zeta$ ,  $\delta$ ,  $\gamma$ ,  $\beta$ ,  $\alpha$  as well as the harmonics and sum/subtraction of fundamental branches. The large Fermi surfaces,  $\eta$ ,  $\epsilon$ ,  $\zeta$ ,  $\delta$ ,  $\gamma$ , correspond to the main Fermi surfaces.

Figure 2 shows the angular dependence of the

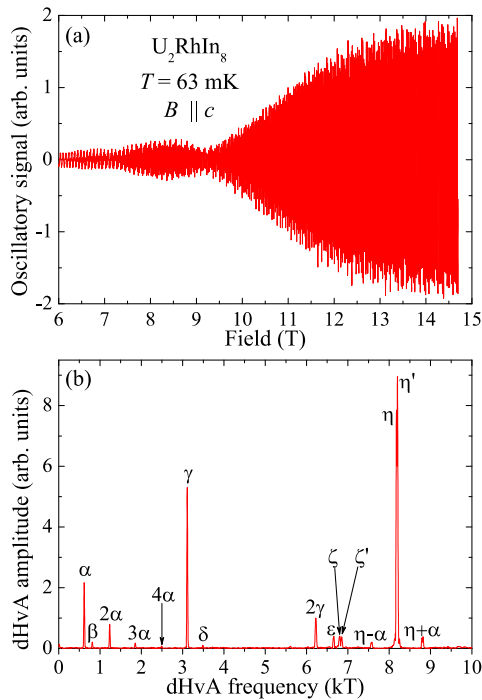


Fig. 1 (a) dHvA oscillations for the field along c-axis in  $U_2RhIn_8$  and (b) the corresponding FFT spectrum



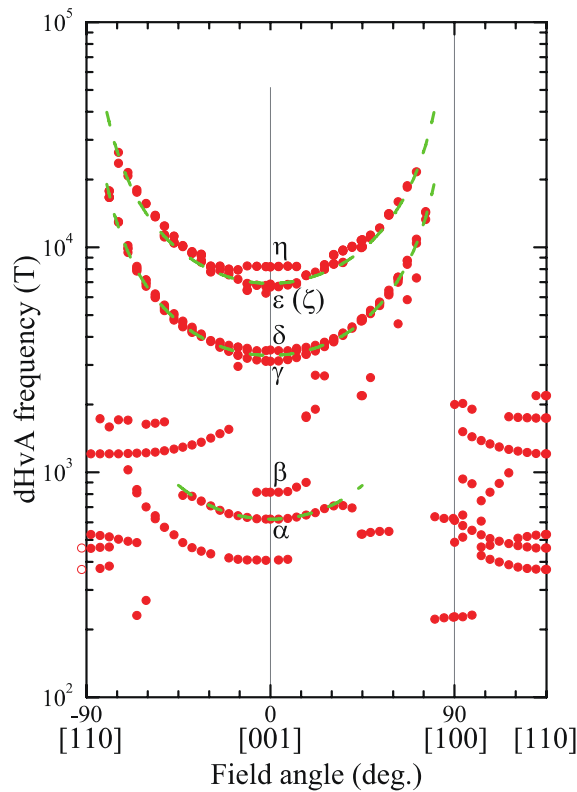


Fig. 2 Angular dependence of the dHvA frequencies in  $U_2RhIn_8$ .

dHvA frequencies. It should be noted that the experiments were done in the antiferromagnetic state, which changes the paramagnetic Brillouin zone into the antiferromagnetic Brillouin zone.

The main dHvA branches,  $\eta$ ,  $\varepsilon$ ,  $\zeta$ ,  $\delta$ ,  $\gamma$ , correspond to two kinds of quasi-two-dimensional Fermi surfaces, in which the frequencies approximately follow  $1/\cos\theta$  dependence. The angular dependence of these frequencies is much larger than those expected in the antiferromagnetic Brillouin zone. Therefore the magnetic breakdown must occur at high fields.

Indeed, according to the band structure calculations, the magnetic breakdown is expected in the Brillouin zone boundaries.

From the temperature dependence of the dHvA amplitude, the cyclotron effective masses are determined for the field along c-axis. The masses are 4.3, 6.8, 6.7, 3.5 and 3.1 $m_0$  for branches  $\eta$ ,  $\varepsilon$ ,  $\zeta$ ,  $\delta$ , and  $\gamma$ , respectively. These values are consistent with the Sommerfeld coefficient, 47 mJ K<sup>-2</sup> mol<sup>-1</sup>, indicating that main Fermi surfaces are detected in this experiment.

This work was done in collaboration with D. Aoki, H. Harima, Y. Homma.

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## Angle-Dependent Magnetoresistance Studies on the Spin-Triplet Superconductor $\text{UTe}_2$

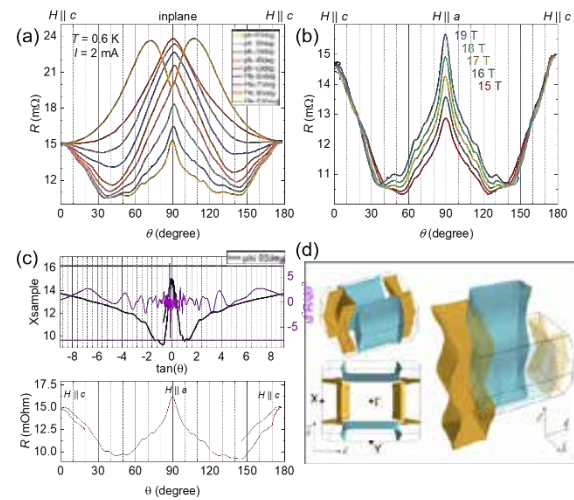
The spin-triplet superconductor  $\text{UTe}_2$  has attracted significant attention recently as a host of various superconducting phases that emerge depending on temperature, pressure, magnetic field strength and orientation. In this project, we explored electric-magnetotransport response of high-quality  $\text{UTe}_2$  single-crystals in magnetic fields up to 25 T at the magnet laboratory of the Institute of Material Research at Tohoku University. We discovered so-called angle-dependent magnetoresistance oscillations originating from a coherent two-dimensional Fermi surface and Shubnikov-de Haas oscillations in the c-axis resistivity that provide deep insights into the electronic properties of  $\text{UTe}_2$ .

Recently found high-field superconducting phases of the heavy-fermion spin-triplet superconductor,  $\text{UTe}_2$ , have been attracting much attention [1-3]. Various distinct field-induced phases, i.e., the field re-entrant superconducting (FRSC) phase for  $B \parallel b$ -axis, and spin-polarized superconducting phase (SPSC) above the metamagnetic transition ( $B_m \sim 35$  T) with  $\sim 30^\circ$  tilted magnetic field from  $b$  to  $c$ , are confirmed. We recently revealed a correlation between the emergence of the SPSC and its upper critical field  $H_{c2}$  and a vanishing anomalous Hall effect (AHE) signal in the angle dependence of  $\text{UTe}_2$  (see Fig. 1a) pointing at a potential compensation mechanism for this exciting high-field phase [4]. To reveal the origin of these field-induced superconducting phases, investigation of electronic properties and their changes induced by magnetic field the field orientation is essential. Especially magnetic quantum oscillations may help to understand the Fermi surface and its relation to the various ground states [5]

High-quality single crystals grown by the molten-flux-flow method are available with superconducting  $T_c$  of 2.1 K. In order to measure electrical transport precisely, we were provided with high quality-single single crystals from Prof. D. Aoki (IMR-Oarai, Tohoku University) optimized for c-axis resistivity measurements. Spot-welding gold leads to the samples achieved low-ohmic contacts. As can be seen in the right panel, we have recently established to fabricate micron-scale transport structures from high-quality single-crystals with ohmic contacts by the help of FIB suitable for magnetotransport experiments.

We ran transport experiments in three different magnet systems, in the all-superconducting 20 T and 15 T magnets as well as in the 25 T hybrid magnet, all equipped with Helium-3 inserts and a 2-axis rotator probe.

As presented in Fig. 1a we recorded the angle-dependent magnetoresistance (AMR)



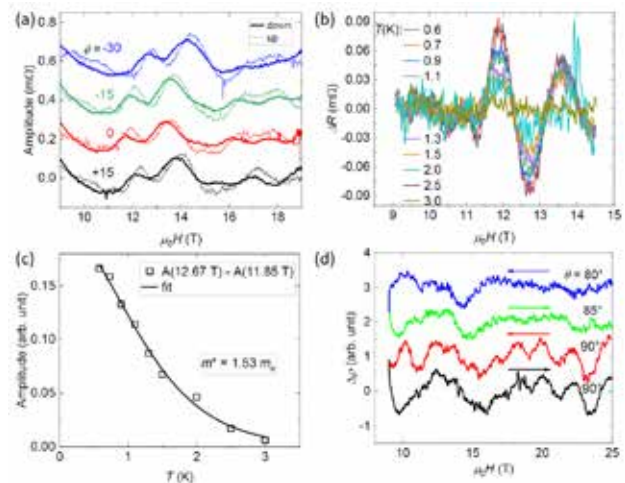
**Fig.1** Angle-dependent magnetoresistance oscillations (AMROs) recorded in the 20 T superconducting magnet with continuously varying  $\theta$  between 0 and  $180^\circ$  ( $\theta = 90^\circ = B \parallel c$ ), (a) at 19 T fixed field for various fixed inplane angles  $\phi$ , (b) at  $\phi = 0^\circ$  (i.e. within the  $a,c$  plane) for various magnetic fields between 15 and 19 T. (c) Comparison of AMROs at  $\phi = 5^\circ$ : (lower panel) Resistance  $R$  versus  $\theta$ , (upper panel)  $R$  and  $d^2R/d\theta$  plotted against  $\tan(\theta)$ . (d) Sketch of the warped 2D Fermi-surface cylinders according to ref. [5].

of the inter-layer (i.e.  $c$ -axis) resistance versus the polar rotation angle,  $\theta$ , recorded at fixed field and various fixed inplane angles,  $\phi$ . For  $\phi = 0^\circ$  clear oscillation-like features are discernible on top of a slowly varying AMR background with a local minimum around  $30 < \theta < 60^\circ$ . A first weak maximum can be spotted at  $50^\circ$  followed by a few more for higher angles. Above  $90^\circ$  a mirrored AMR is found (expected from the orthorhombic crystal symmetry). We were able to check these AMROs for different angles and fields (Fig. 1b). The semi-classical AMROs are expected to be periodic in  $\tan\theta$ . This is confirmed by the comparison in Fig. 1c. The observed AMRO confirm the presence of

warped 2D Fermi-surface cylinders in the band structure of  $\text{UTe}_2$ . We are currently analyzing these data and a publication is underway.

As can be seen in Fig. 2a slow Shubnikov-de Haas (SdH) oscillations with a frequency of approximately 90 T in the c-axis magnetoresistance were observed for the field oriented along the  $a$ -axis. This direction is perpendicular to the orientation of the 2D Fermi surface cylinders responsible for the AMROs shown above. We were able to trace these oscillations for different angles within the  $a,b$ - and the  $a,c$ -planes (see Fig. 2a, b and d, respectively). The low frequency indicates a very small cyclotron orbits associated with a small Fermi surface. The value is incompatible with the large cylinders reported previously from de Haas-van Alphen oscillation measurements [6]. Such a small oscillation frequency may originate from a small 3D Fermi surface suggested from previous photo-emission experiments [7] and high-field tunnel-diode-oscillator experiments [8]. From the temperature dependence of the oscillation amplitude (shown in Fig. 2b and c) we extracted a rather light effective mass of about 1.5 times the free electron mass,  $m_e$ . This low value matches previous reports in ref. [5], where such a small cyclotron orbit was associated with quantum interference oscillations between electron- and hole-like 2D-Fermi-surface cylinders. We were able to trace the oscillations up to inplane angles of about  $45^\circ$ . In the  $a,c$ -plane the oscillations disappeared rather quickly already within only a few degrees away from the  $B \parallel a$  direction. We are currently analyzing the observed data and are trying to compare them to band-structure calculations. An additional publication is underway. Therefore, our observations provide extremely valuable insights into the electronic properties of  $\text{UTe}_2$ .

In summary, we were able to observe angle-dependent magnetoresistance oscillations and the Shubnikov de Haas effect in the c-axis resistivity of single crystalline  $\text{UTe}_2$ . The comprehensive studies of the effects depending on field, field orientation, and



**Fig. 2** SdH oscillations after subtraction of an O(2) polynomial fit (a) for different inplane angles  $\phi$  (within the  $a,b$  plane), recorded in the 20 T superconducting magnet (b) for different temperature, recorded in the 15 T superconducting magnet. (c) Effective-mass plot: Oscillation amplitude at 12.26 T for various temperatures ranging from 0.6 to 3 K. (d) SdH oscillations recorded in the 25 T hybrid magnet for three different polar angles  $\theta$  (within the  $a,c$  plane).

temperature has resulted in a profound understanding of the electronic ground state in  $\text{UTe}_2$ . Experiments at even higher fields are highly desirable in order to learn more about the evolution of the Fermi surface, potentially also once the system transitions into the high-field spin-polarized phase above the metamagnetic transition field  $B_m \sim 35$  T. In the future we would also like to study Hall effect and quantum oscillations at dilution temperatures in order to learn more about  $\text{UTe}_2$ .

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Keywords: Fermi surface, magnetoresistance, superconducting

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## Link between high field reentrant superconductivity and multiple superconductivity under pressure in $\text{UTe}_2$

We conducted AC calorimetry measurements under high magnetic fields and pressure on the spin-triplet superconductor  $\text{UTe}_2$ . With increasing pressure, the field-reentrant superconducting phase observed at ambient pressure for the field along the b-axis shifts to a lower field and higher temperature region, revealing double superconducting transitions at high pressure. These results indicate that the high-field reentrant superconducting phase is identical to the high-temperature superconducting phase under pressure.

Recent discovery of superconductivity in  $\text{UTe}_2$  attract much attention, because of its unusual superconducting properties.  $\text{UTe}_2$  is a heavy fermion paramagnet with the Sommerfeld coefficient  $\gamma \sim 120 \text{ mJ K}^{-2} \text{ mol}^{-1}$ . It crystallizes in the orthorhombic structure with the space group  $Immm$ . Although it is a body-centered structure, the inversion center is not located at the atomic site, meaning that the local inversion symmetry is broken. Superconductivity occurs at  $T_c = 1.6\text{--}2.1 \text{ K}$ . It had been suggested that  $\text{UTe}_2$  is an end member of ferromagnetic superconductors,  $\text{UCoGe}$ ,  $\text{URhGe}$ , and  $\text{UGe}_2$ . The ferromagnetic fluctuations are, however, not experimentally established, while the antiferromagnetic fluctuations with an incommensurate wave-vector is detected by the inelastic neutron scattering

experiments.

The huge superconducting upper critical field  $H_{c2}$  and the multiple superconducting phases are a strong support for the spin-triplet state of superconductivity in  $\text{UTe}_2$ . When the field is applied along the b-axis, which is a hard-magnetization axis, the  $H_{c2}$  curve shows the field-reentrant behavior above 15T, and it continues up to 35T, at which the first order metamagnetic transition occurs. The superconducting phase is abruptly suppressed above 35T.

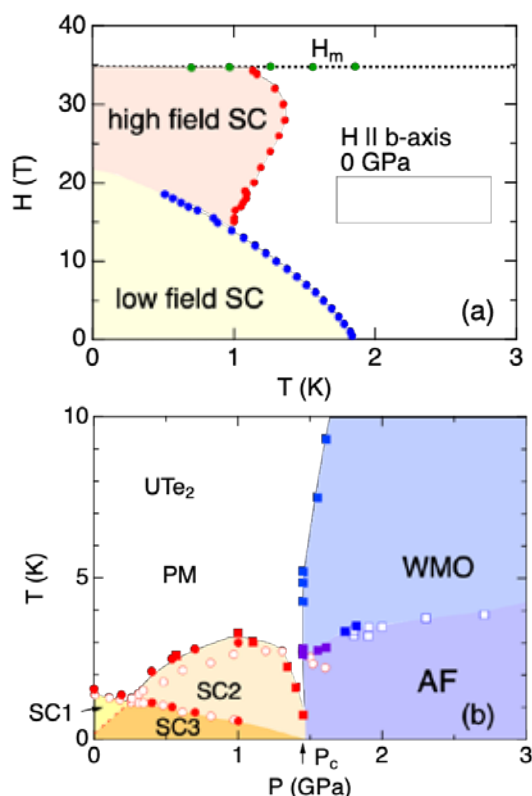


Fig. 1 (a) H-T phase diagram for the field along b-axis at ambient pressure in  $\text{UTe}_2$ . (b) T-P phase diagram at zero field.



Fig. 2 Photograph of a miniature pressure cell placed on the horizontal rotator for PPMS

As shown in Fig.1(a), our recent specific heat measurements [1] reveals that there is a phase boundary between the field-reentrant superconductivity and low-field superconductivity, indicating multiple superconducting phases as thermodynamic evidence.

On the other hand, the multiple superconductivity is initially found under pressure through our AC calorimetry measurements [2,3]. As shown in Fig.1(b), with increasing pressure,  $T_c$  splits at relatively low pressure,  $\sim 0.2 \text{ GPa}$ . The low temperature  $T_c$  continuously decreases, while the high temperature  $T_c$  increases, reaching a broad maximum,  $T_c \sim 3 \text{ K}$  at around  $1 \text{ GPa}$ , and then decreases. At the critical pressure,  $P_c \sim 1.5 \text{ GPa}$ , superconducting phases are abruptly suppressed, and the antiferromagnetic state is realized.

It is important to study this rich phase diagram through a thermodynamic method



with fine tuning pressure, field direction using high quality single crystals. In this study, we performed the AC calorimetry measurements for the field along the b-axis under pressure.

Our first target is to develop a miniature pressure cell, which can be rotated at high fields and at low temperatures. Figure 2 shows a photograph of our miniature pressure cell, which is placed on the horizontal axis rotator for PPMS. The first attempt to generate pressure was successful. As a 2nd step, we are now testing the pressure cell with a  $\text{UTe}_2$  sample for AC calorimetry measurements.

We also performed the AC calorimetry measurements under pressure using a conventional piston cylinder cell for the field along the b-axis. Figure 3(a) shows the temperature dependence of the AC calorimetry under pressure at 0.15 GPa at different fields for  $H \parallel b$ -axis. A sharp specific heat jump due to superconductivity is observed at zero field. At high fields above 8 T, in addition to the sharp specific heat jumps, broad transitions appears at higher temperatures, indicating the high field superconducting phase under magnetic fields.

Further increasing the pressure, high field superconducting phase shifts to lower field region, and finally double superconducting transitions are observed at zero field.

Our results suggest that high field superconducting phase at ambient pressure is identical to the high temperature superconducting phase under pressure. The evolution of the multiple superconducting phases at high fields and at pressure was demonstrated.

This work was done in collaboration with T. Vasina, D. Aoki.

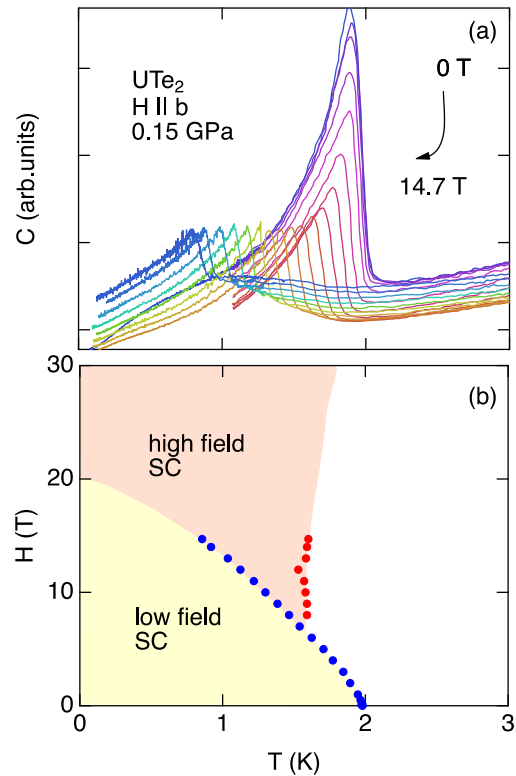


Fig. 3 (a) Temperature dependence of AC calorimetry at different fields for  $H \parallel b$ -axis under pressure at 0.15 GPa. (b) H-T phase diagram at 0.15 GPa for  $H \parallel b$ -axis.

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Keywords: Superconductivity, high pressure, spin-triplet  
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## Porous metal-intermetallic composites by liquid metal dealloying

Nanoporous metals with a bicontinuous structure, produced by liquid metal dealloying (LMD), are regarded as promising materials for energy-related applications because of their good electrical conductivity, mass transportability, and bulk specimen formability by the top-down process, that are distinct from other nanomaterials. Here, we explore synthesis of porous metal-intermetallic composites as promising hybrid battery electrode materials combining open porous metallic collector and TiSi-based active material.

Liquid metal dealloying is a metallurgical method for the synthesis of open porous materials established by Kato and co-workers [1-2]. Liquid metal dealloying implies selective removal of one or more elements from a multi-element precursor material by a reactive liquid metal during its contact with this liquid metal. The remaining elements of the precursor material rearrange themselves into an open porous structure.

The selection of materials for liquid metal dealloying is based on the free energy change during mixing of elements  $\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}$ , where  $\Delta H_{mix}$  is the heat of mixing,  $\Delta S_{mix}$  is the entropy of mixing, and  $T$  is the absolute temperature. Usually, the entropy  $\Delta S_{mix}$  increases after mixing. So, from a thermodynamic point of view, if  $\Delta H_{mix} < 0$ , the  $\Delta G_{mix} < 0$ , and the mixing reaction can occur spontaneously. Thus, the precursor material should consist of elements having high positive and high negative heat of mixing  $\Delta H_{mix}$  with liquid metal.

In this work, four precursor  $(\text{TiCu})_{100-x}\text{Si}_x$  at% alloys, where  $x=1, 5, 10, 20$  at%, have been synthesized using an arc-melter.

The heat of mixing  $\Delta H_{mix}$  between both couples Mg and Cu (-3 kJ/mol) as well as Mg and Si (-26 kJ/mol) is negative. The heat of mixing  $\Delta H_{mix}$  between Mg and Ti (16 kJ/mol) is positive. Therefore, it is expected that Cu and Si will be dissolved into Mg during liquid metal dealloying. The remaining Ti is expected to be rejected by liquid magnesium and rearranged into an open porous structure. However, our experimental results demonstrate that Si in the presence of Ti is rejected by Mg. This is likely due to a very high negative enthalpy of mixing between Ti and Si (-66 kJ/mol).

The as-arc-melted  $(\text{TiCu})_{50-x}\text{Si}_x$  precursor samples were cut into 1 mm thick samples which were subjected to liquid metal dealloying, namely, immersed in liquid Mg (Fig. 1). The dealloying conditions are 1073 K and 20 min. After liquid metal dealloying, the evolved pores were naturally filled with magnesium. Mg was chemically removed by immersing as-dealloyed samples into 3M aqueous solution of nitric acid for 5 h (Fig. 1).

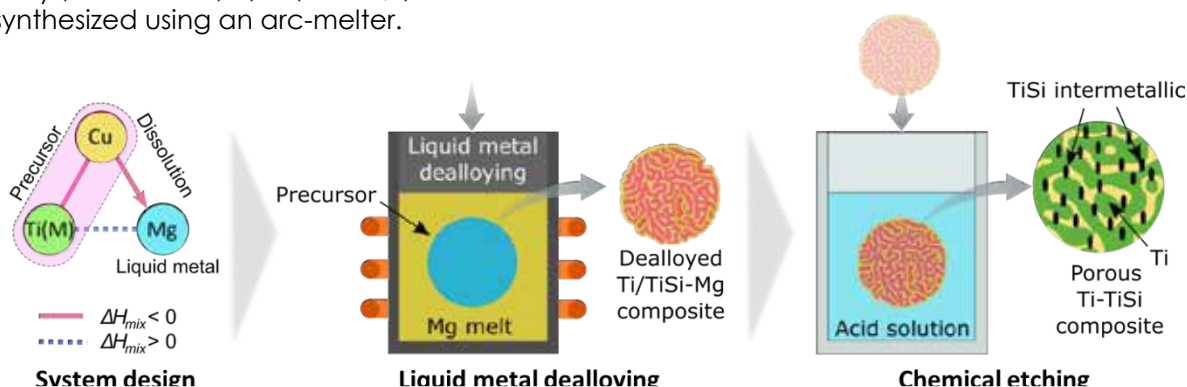


Fig. 1 Schematic illustration of the synthesis of porous metal-intermetallic composites by means of liquid metal dealloying and chemical etching.



Fig. 2 shows the microstructure of the  $(\text{TiCu})_{50-x}\text{Si}_x$  at% samples after liquid metal dealloying and chemical etching. According to the microstructural analysis, the porous samples mainly consist of two phases. These are Ti and TiSi-based intermetallic phases. The TiSi-based phase contains about 30 at% of Si as detected by EDX-SEM. The volume fraction of the TiSi-based phase significantly increases with the increasing Si concentration in the precursor alloys. At  $x=1$  at%, the microstructure of the open porous metal-intermetallic composite consists of  $\mu\text{m}$ -scale Ti ligaments covered by TiSi-based ligaments of a few hundred nanometers.

At  $x=5$  at%, large crystals of the TiSi-based intermetallic phase, approximately  $10\ \mu\text{m}$  in cross-section, are observed instead of nm-scale TiSi-based ligaments. At  $x=10, 20$  at%, the volume fraction as well as size of those TiSi-based crystals increases. Specifically, at  $x=20$  at%, the crystals reach a few tens of  $\mu\text{m}$  in cross section. Furthermore, the faceting of the TiSi-based crystals becomes more pronounced.

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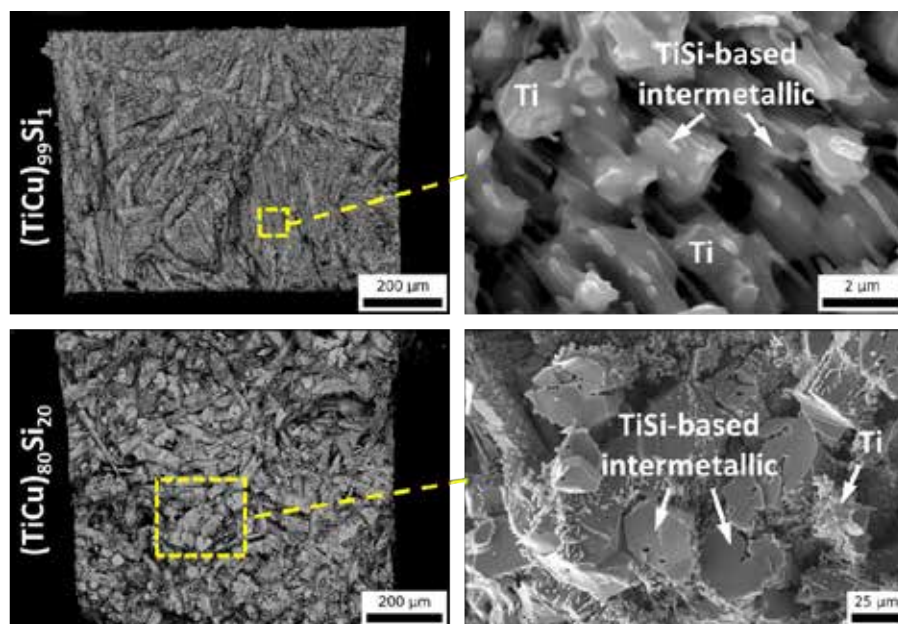


Fig. 2 Secondary electron micrographs of porous Ti-TiSi composites obtained from  $(\text{TiCu})_{99}\text{Si}_1$  (top panel) and  $(\text{TiCu})_{80}\text{Si}_{20}$  (bottom panel) at%.

### Keywords: Porosity

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## Fabrication of 3D interconnected dual-phase heterostructures in CoCrFeMnNi high entropy alloy using the Liquid Metal Dealloying process with Cu melt

The dealloying reaction between a CoCrFeMnNi high-entropy alloy (HEA) precursor and molten Cu at 1095°C was investigated as a function of immersion time. EDX mapping and line analyses revealed that Mn and Ni, which have high reactivity with Cu, were the first to undergo dealloying reactions in the CoCrFeMnNi HEA precursor. Consequently, Cu-rich melt channels penetrated the precursor alloy, forming a unique 3D interconnected heterostructure.

There have been wide variety of developments for 3D interconnected materials using dealloying techniques. In general, dealloying is referred to a corrosion phenomenon in which the more active element is selectively removed from an alloy under certain environmental conditions. The liquid metal dealloying (LMD) process, which is different from chemical dealloying and vapor dealloying, has also been actively studied for a decade. In 2011, Wada et al. first reported this novel dealloying process to develop the 3D interconnected non-noble materials [1]. The LMD process is based on the miscibility relationship between the constituent elements of precursor alloy and a liquid metal [2-5]. Liquid metal is utilized as a dealloying medium, and it selectively takes out miscible elements from a precursor alloy. The selective dissolution results in interface diffusion of immiscible atoms, and the self-organization phenomenon of immiscible atoms into 3D interconnected morphology is involved. Simultaneously, the liquid melt penetrates the precursor material, and the 3D interconnected melt channels are formed due to the LMD reaction.

Previous LMD studies have focused on simple LMD systems where thermodynamic reactions can be easily predicted by miscibility relationships among elements of precursor alloy and metallic melt. However, this study aims to fabricate a new heterostructure microstructure by using a high-entropy alloy (HEA) composed of more than five principal elements as the precursor.

The CoCrFeMnNi HEA, known for its excellent mechanical properties at cryogenic temperatures, was homogenized at 1100 °C for 6 h, then cold-rolled with a 75% reduction and recrystallized at 1050 °C to prepare the precursor alloy. Holes were then machined into the specimens, and they were immersed in molten copper at 1095 °C for 2, 5, 10, and 12 min using a W wire.

The microstructure produced by LMD

exhibited a complex 3D interconnected heterostructure, distinct from the typical dendritic cast structures or equiaxed recrystallized microstructures (Fig. 1). The thickness of the dealloyed reaction layer was measured at 228, 453, 766, and 708 μm for immersion times of 2, 5, 10, and 12 min, respectively. After 12 min of the LMD process, the entire specimen transformed into a 3D interconnected composite, indicating a significantly faster reaction rate compared to other metallic melts such as Mg.

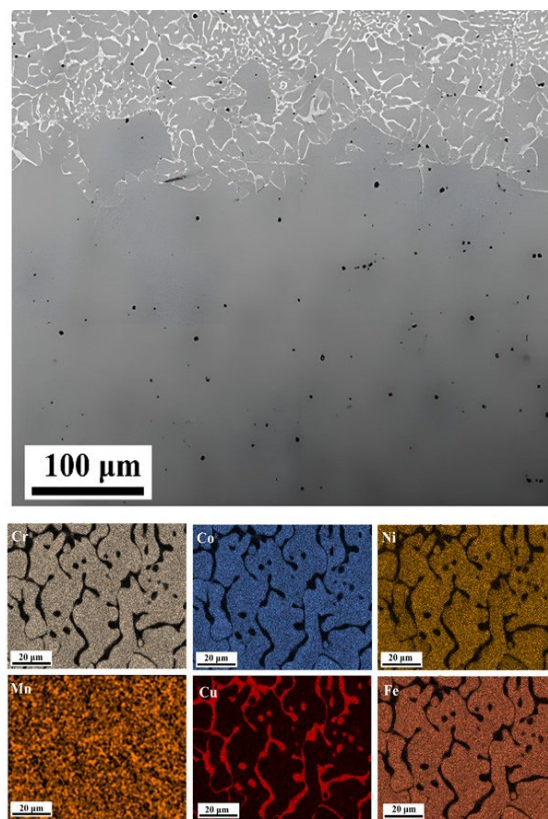


Fig. 1 Heterostructure developed by the LMD process using a CoCrFeMnNi precursor with Cu melt.

The fabricated heterostructure composite was formed by the self-organization phenomenon of the solid ligament phase and Cu-rich melt channels during the LMD process, as confirmed by EDS maps showing a 3D interconnected structure (Fig. 1). In the solid ligament phase, Cr, Co, and Fe were uniformly distributed, and a small amount of Cu (6.6 at.%) was also alloyed. In the Cu-rich melt channel region, Mn and Ni were dissolved around 5 at.% with small amounts of Cr, Co, and Fe also reacting and present in the melt channel. Based on the measured compositions, the mixing entropy was calculated, showing that the solid ligament phase exhibited a mixing entropy of 1.79R, characteristic of a HEA, while the Cu-rich melt phase exhibited a mixing entropy of 1.32R, indicating characteristics of a medium-entropy alloy.

To investigate the diffusion behavior and self-organization phenomena between the CoCrFeMnNi HEA precursor and Cu melt, a line EDS analysis was conducted (Fig. 2). The right graph shows that Mn and Ni were initially dissolved and detected in the Cu melt, with Mn being almost entirely dissolved and some Ni remaining in the solid ligament. Additionally, unlike previous LMD reactions where the melt's elements did not dissolve into the solid ligament, this study observed a significant amount of Cu alloying.

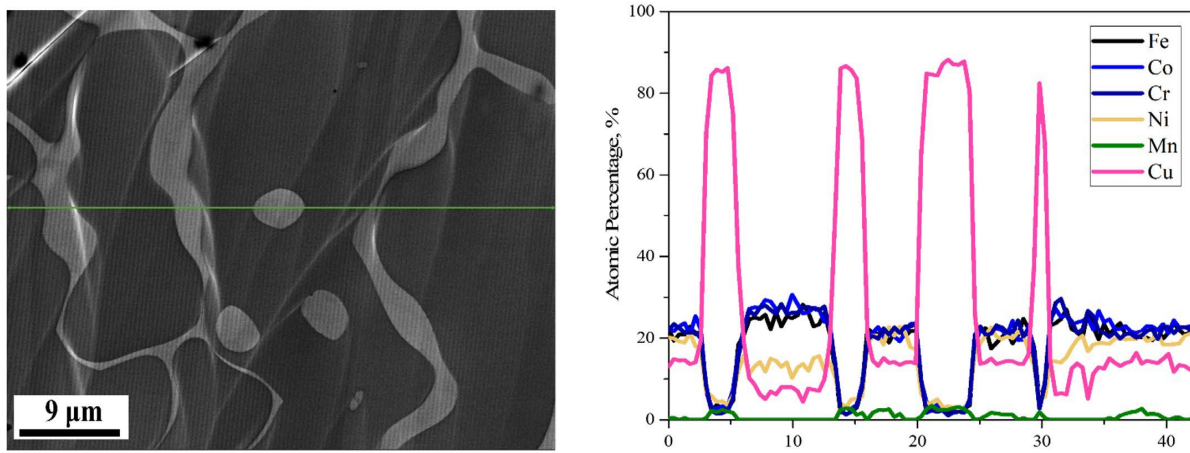


Fig. 2 Line EDX analysis results along the green line (left) crossing the solid ligament and Cu-rich melt phase regions.

Keywords: 3D structure, metal, diffusion  
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Activity Report

Workshops



## Workshops

| No.     | Chairperson or Committee Member | Title of Workshop                                                                                                                                                                                       | Place            | Term                  |
|---------|---------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|-----------------------|
| 23WS1   | Prof. Fujita                    | GIMRT Workshop: Resonant Inelastic and Elastic X-ray Scattering (RIXS/REXS)                                                                                                                             | Sendai           | 2023.8.2-2023.8.4     |
| 23WS2   | Prof. Nojiri                    | GIMRT Workshop: Reimei-GIMRT Workshop "Quantum Beams Study of the Dynamics of Rare Earth Garnets"                                                                                                       | Sendai           | 2023.8.7-2023.8.8     |
| 23WS3   | Prof. Kato                      | GIMRT Workshop: The 18th International Workshop on Biomaterials in Interface Science                                                                                                                    | Sendai           | 2023.8.4              |
| 23WS4   | Prof. Orimo                     | GIMRT Workshop: The 7th Symposium for the Core Research Clusters for Materials Science and Spintronics, The 6th Symposium on International Joint Graduate Programs in Materials Science and Spintronics | Sendai           | 2023.11.28-2023.12.1  |
| 23KW    | Prof. Aoki                      | ICC Workshop: KINKEN WAKATE 2023: International Materials Science School 2023-Advances in Strongly Correlated Electron Systems                                                                          | Grenoble, France | 2023.10.9-2023.10.12  |
| SMS2023 | Prof. Sasaki                    | Summit of Materials Science 2023 and GIMRT User Meeting 2023                                                                                                                                            | Sendai           | 2023.11.20-2023.11.22 |



## Workshop on Resonant Inelastic and Elastic X-ray Scattering

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Keywords: Resonant Inelastic Scattering, Resonant Elastic Scattering

Workshop on Resonant Inelastic and Elastic X-ray Scattering was held at Sakura Hall, Tohoku University in August 2–4, 2023. We had over 100 participants, including 35 from overseas. The program featured 5 plenary talks, 15 invited talks, 11 contributed talks, and 20 poster presentations. On the final afternoon, we organized a NanoTerasu tour, which attracted about 60 participants. Throughout the workshop, there were active discussions and meetings on collaborative research, with a focus on new beamlines at NanoTerasu. The workshop ended on a positive note, with attendees showing keen interest and active involvement throughout.

### 1. 緒言 (Introduction,)

共鳴非弾性および弾性 X 線散乱 (RIXS および REXS) は、いずれも X 線散乱の原理に基づいた実験手法である。RIXS は、非弾性散乱に注目して物質中の低エネルギー励起を明らかにし、REXS は弾性散乱に注目して回折現象を通じて物質中の周期構造を明らかにする。

RIXS は、結晶場、軌道間励起 (*dd* 励起、*ff* 励起など)、電荷移動励起などの電子状態そのものを反映する低エネルギー励起だけでなく、固体中の磁気励起 (マグノン) やフォノン、分子系の振動励起の観測も可能である。エネルギーだけでなく、X 線の運動量を利用することによって素励起の分散を取得することができる。さらに、*photon-in/photon-out* の分光なので、バルク敏感であり、様々な相 (固体、液体、気体) や様々な外場 (電場、磁場、応力) においても電子状態を測定できることから、*operando* 分光に強みを持つなど、RIXS は他に類を見ない強力な分光手法となっている。

一方、REXS は回折に基づいた手法であるが、従来の X 線回折で研究できる結晶構造を調べられるだけでなく、共鳴効果による散乱断面積の増強を利用して、物質中のスピンや電荷、軌道の空間変調も観察可能であり、これにより、REXS もまた他に類を見ない強力な回折の実験手法となっている。

これらの 2 つの実験手法は同じ散乱の原理に基づいているが、RIXS は分光法として、REXS は回折法として、異なる計測技術として発展してきた。そのため、RIXS と REXS の研究は、理論も含め別々に発展してきたが、X 線散乱という共通の現象から物質研究に必要な電子状態と構造の両方の情報を取得できる点で、完璧な組み合わせと言える。近年は放射光光源や実験技術の向上により、RIXS と REXS の装置の違いが小さくなっており、特に、RIXS 分光器を使用して回折を測定する有用性が認識されるようになったことから、統一的な理解とさらなる融合研究が期待されている。

そこで、先進的な共鳴 X 線散乱法および関連する理論技術を使用して量子材料、磁性、電子秩序、および励起を研究する研究者が集い、議論する場を提供し、両手法の融合的な研究、統一的な理解を目指して、本ワークショップを開催する。対象となる物質は、遷移金属酸化物、銅酸化物・鉄系超伝導体、希土類系、強いスピン軌道相互作用を有する系、ヘテロ構造などが含まれる。

本ワークショップは 2 年おきに開催されており、最近では、2016 年に IFW Dresden で、2018 年に Diamond Light Source で、2021 年には (Covid-19 の影響により 1 年延期された) Brookhaven National Laboratory で開催されている。2023 年の開催では、建設中の NanoTerasu での共同研究を視野に入れて、仙台の地で開催することとした。

## 2. 開催内容 (Experimental procedure)

本ワークショップは、2023 年 8 月 2-4 日に、東北大学片平キャンパスさくらホールにて、東北大学 金属材料研究所と量子科学技術研究開発機構 次世代放射光施設整備開発センターの共同主催で開催した。一部の海外の発表者を除き、対面形式で実施した。

プログラムは大きく分けて 5 つのセッションに分かれ、各セッションに最近の研究動向を概観する plenary talk と、関連する注目度の高い研究テーマに関する invited talk を配置した。さらに、参加者からの興味深い研究成果を contributed talk として取り上げ、RIXS/REXS に関連する実験・理論的手法を用いた量子物質や磁性、電子秩序、励起状態に関する最近の研究を広く網羅する形とした。また、ポスター発表のセッションも設け、より多くの参加者に発表、議論の場を提供することとした。最終日の午後には、世界最高の性能を目指す RIXS 装置を含む新たなビームラインが建設中である NanoTerasu の見学会を実施した。

図 1、図 2 に口頭及びポスター発表のプログラムを示す。発表件数は、plenary talk が 5 件、invited talk が 15 件、contributed talk が 11 件、ポスター発表が 20 件であった。

| RIXS/REXS Workshop 2023 – Program (final) |                                                                                                                                                                                                             |                      |                                                                                                                                                                                                              |
|-------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Wednesday, August 2nd                     |                                                                                                                                                                                                             | Thursday, August 3rd |                                                                                                                                                                                                              |
| Registration                              |                                                                                                                                                                                                             | Registration         |                                                                                                                                                                                                              |
| 9:00-9:20                                 | Opening Remarks (Chair: Masaki Fujita (Tohoku University))<br>Dr. Wataru Usui, Director of AIST, QST<br>Prof. Takahiko Banai, Director of RRI, Tohoku University                                            | 9:00-9:45            | Mark P. M. Dean (Brookhaven National Laboratory)<br>Electronic structure, magnetic interactions, and charge order in low-carbon materials<br>Invited by RRI                                                  |
| 9:20-10:05                                | Xi-Jin Zhou (Diamond Light Source)<br>Spin and charge excitations in quantum materials probed by RIXS                                                                                                       | 9:45-10:15           | Yao Wang (Cambridge University)<br>Manipulation of Magnet, Excitations and Entanglement Entangled by RIXS                                                                                                    |
| 10:05-10:35                               | Johann Chang (University of Zurich)<br>Magnet-magnon interactions in 2D ferromagnetic insulators                                                                                                            | 10:15-10:45          | Azusa Hara (Osaka Metropolitan University)<br>Manipulation of Magnet, Excitations and Entanglement Entangled by RIXS                                                                                         |
| 10:35-11:05                               | Yingying Peng (Peking University)<br>Charge order and its dynamics in intercalated cuprates                                                                                                                 | 10:45-11:15          | Break                                                                                                                                                                                                        |
| 11:05-11:35                               | Break                                                                                                                                                                                                       | 11:15-11:45          | Naoki Suzuki (Max-Planck-Institut, Tohoku University)<br>Controlled spin and orbital dynamics in 3d/5d Mott insulators                                                                                       |
| 11:35-12:05                               | Qi-Jing Huang (National Synchrotron Radiation Research Center)<br>Electronic excitations of cuprate superconductors probed with high-resolution RIXS                                                        | 11:45-12:05          | Naoya Isikawa (Chiba University)<br>Controlled excitations in quantum magnet: spin scattering spectra of spin-1/2 Mott insulators                                                                            |
| 12:05-12:25                               | Wengui Tanaka (National Institute for Materials Science)<br>Phonon scattering and phonons in cuprate superconductors                                                                                        | 12:05-12:25          | Subhayan Roychowdhury (Lawrence Berkeley National Laboratory)<br>Quantum A-Bit and quantum first principles method for the simulation and analysis of quantum materials using scattering                     |
| 12:25-13:30                               | Lunch                                                                                                                                                                                                       | 12:25-13:30          | Lunch                                                                                                                                                                                                        |
| 13:30-14:30                               | Poster session                                                                                                                                                                                              | 13:30-14:30          | Poster session                                                                                                                                                                                               |
| 14:30-15:15                               | Ugo Stroob (Paul Scherrer Institute)<br>Resonant scattering to study orbital dynamics of spin and electronic and the magnetic order dynamics of the LaNiO <sub>3</sub>                                      | 14:30-15:15          | Munen Mizuno (Harvard University)<br>Towards a quantum spin description of spin-driven quantum magnetism                                                                                                     |
| 15:15-15:45                               | Takayoshi Kimura (University of Tokyo)<br>Orbital-ordered magnetism and the effect of multiorbital Co <sup>2+</sup>                                                                                         | 15:15-15:45          | Giacomo Coslovich (SLAC National Accelerator Laboratory)<br>Orbital Resonant X-ray Scattering Reveals Light-enhanced Charge Density Wave Coherence in cuprate Bi <sub>2</sub> Se <sub>3</sub> Superconductor |
| 15:45-16:15                               | William Windsor (First Nano Institute of the Max Planck Society)<br>Towards control of orbital spin dynamics in 4d ultrathin magnets                                                                        | 15:45-16:15          | Nicolas Jeevan (Synchrotron SOLEIL)<br>Magnetic chirality in multilayers probed by X-ray magnetic scattering                                                                                                 |
| 16:15-16:45                               | Break                                                                                                                                                                                                       | 16:15-16:45          | Break                                                                                                                                                                                                        |
| 16:45-17:15                               | David Hawthorn (University of Waterloo)<br>Orbital-magnetism and Charge Density Wave Order in Cuprate Superconductors Probed by Resonant Elastic X-ray Scattering                                           | 16:45-17:15          | Eugenio Parisi (Paul Scherrer Institute)<br>Orbital Dynamics in Spinless Magnet Using Time-resolved Resonant Inelastic X-ray Scattering at Resonant X-ray                                                    |
| 17:15-17:35                               | Hao-Yu Huang (National Synchrotron Radiation Research Center)<br>Resonant inelastic x-ray scattering of charge order in La <sub>1-x</sub> Bi <sub>x</sub> FeO <sub>4</sub> revealed by high-resolution RIXS | 17:15-17:35          | Kengo Tsutsui (QST)<br>Theoretical study of magnetic excitations in a photoinduced Mott insulator on a square lattice                                                                                        |
| 17:35-17:55                               | Wen Garcia-Fernandes (Diamond Light Source)<br>Low energy orbital excitations in A-site ordered SrBi <sub>2</sub> Se <sub>2</sub> O <sub>9</sub>                                                            | 17:35-17:55          | Vivek Kumar Shrivastava (Brookhaven National Laboratory)<br>Superconducting signature of 4d magnetism in a van der Waals ferromagnetic Perovskite                                                            |
| 18:30-20:30                               | Workshop Dinner                                                                                                                                                                                             | 18:30-20:30          | Workshop Dinner                                                                                                                                                                                              |

図 1 ワークショップのプログラム。

| Poster Presentation List |                      |                                                                  |                                                                                                                                                                                                    |
|--------------------------|----------------------|------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                          | Presenter            | Affiliation                                                      | Title                                                                                                                                                                                              |
| 1                        | Asakura, Daisuke     | National Institute of Advanced Industrial Science and Technology | Transition-metal L-edge RIXS studies of cathode materials for Li-ion batteries: Relation between the charge-transfer effect and electrode performance                                              |
| 2                        | Fujii, Kentaro       | National Institutes for Quantum Science and Technology           | Cu L-edge RIXS Spectra of Cu-Proteins                                                                                                                                                              |
| 3                        | Fujiwara, Hidenori   | Osaka University                                                 | Probing spin-polarized electronic structures of halfmetallic Heusler alloys using RIXS-MCD                                                                                                         |
| 4                        | Geprägs, Stephan     | Walther-Meißner-Institut                                         | Control of magnetic properties in iridate thin films by variation of strain and thin film thickness                                                                                                |
| 5                        | Horio, Masafumi      | University of Tokyo                                              | Comparative RIXS investigation of five- and six-fold oxygen-coordinated 214-type cuprates                                                                                                          |
| 6                        | Jia, Xun             | Chinese Academy of Sciences                                      | Orbital excitations on the cusp of Mott-band insulator crossover in 1T-TaS <sub>2</sub>                                                                                                            |
| 7                        | Juhin, Amélie        | IMPMC-CNRS                                                       | Magnetic properties of binary ferrofluids investigated by RIXS-MCD spectroscopy                                                                                                                    |
| 8                        | Li, Hao              | University of Tokyo                                              | The role of oxygen species on water uptake by hydrophobic materials                                                                                                                                |
| 9                        | Miyawaki, Jun        | National Institutes for Quantum Science and Technology           | Construction of Ultrahigh Energy Resolution 2D-RIXS at NanoTerasu: Advancements and Current Progress                                                                                               |
| 10                       | Nakata, Suguru       | University of Hyogo                                              | Charge order in cuprates revealed by resonant inelastic x-ray scattering                                                                                                                           |
| 11                       | Onishi, Hiroaki      | Japan Atomic Energy Agency                                       | Spin quadrupole excitations in frustrated ferromagnetic chain                                                                                                                                      |
| 12                       | Soh, Jian-Rui        | Ecole Polytechnique Federale Lausanne                            | Entangled spin-orbital-lattice order in Ba <sub>2</sub> MgReO <sub>6</sub>                                                                                                                         |
| 13                       | Takahashi, Yoshihiro | Osaka Metropolitan University                                    | LDA+DMFT approach to resonant inelastic x-ray scattering in strongly correlated magnetic systems                                                                                                   |
| 14                       | Thomas-Hunt, Jack    | Aarhus University                                                | High resolution spin texture imaging in spin caloritronics device structures: New opportunities for REXS at 4th generation light sources.                                                          |
| 15                       | Tomasello, Bruno     | University of Kent                                               | Role of magneto-crystalline anisotropies in complex rare-earth garnets                                                                                                                             |
| 16                       | Tomiyori, Yusuke     | University of Tokyo                                              | The Study on Water Repellent Behavior of Hydrophobic Coatings by Soft X-ray Spectroscopy                                                                                                           |
| 17                       | Yamaguchi, Tatsuya   | Osaka Metropolitan University                                    | Cu L <sub>3</sub> -edge resonant inelastic x-ray scattering on isostructural copper oxides CaCu <sub>3</sub> Fe <sub>4</sub> O <sub>12</sub> and EuCu <sub>3</sub> Fe <sub>4</sub> O <sub>12</sub> |
| 18                       | Yamasaki, Yuichi     | National Institute for Materials Science                         | Anisotropic Magnetic Dipole Detectable by Resonant X-ray Scattering                                                                                                                                |
| 19                       | Zhang, Yujun         | Chinese Academy of Sciences                                      | Hard X-ray High Energy Resolution Spectroscopy Beamline at High Energy Photon Source                                                                                                               |
| 20                       | Su, Jia-Syuan        | National Yang Ming Chiao Tung University                         | Momentum-resolved RIXS studies on high-temperature superconductor Bi2212                                                                                                                           |

図 2 ポスター発表のリスト

### 3. 成果 (Results)

参加者は合計で 100 名以上と非常に多く、海外からの参加者も 35 名程度（オンライン発表の 4 名を含む）と積極的な参加があった。図 3 に参加者の集合写真を示す。1 日目午前と 2 日目午前の plenary talk では、DLS、NSLS-II にある最新の超高分解能 RIXS 装置での成果を含む固体中の素励起に関する最新の研究動向に関する発表があり、続く invited/contributed talk では、SLS、ESRF、DLS、NSLS-II、TPS などの高分解能 RIXS 装置での成果が銅酸化物超伝導体や Fe 超伝導体などを中心に発表された。3 日目午前の plenary talk では、ALS における in-situ や operando RIXS の展開について発表があり、RIXS のユニークな性能を活用した路線も注目を集めた。1 日目午後、2 日目午後の plenary talk では、REXS に関する最新の研究動向に関する発表があり、続く invited/contributed talk を含め、XFEL を用いた時間分解 RIXS/REXS の大きな進展が話題の中心であった。ポスター発表では、企業展示もあり、活発かつ深い議論が各所に見られた。全体を通じて、2 日半にわたるワークショップでは、常時 70 名以上の参加者があり非常に盛況であった。

最終日の午後には NanoTerasu の見学会を実施し、約 60 名の参加者があった。NanoTerasu では、BL02U で世界最高の分解能を目指す超高分解能 RIXS が建設中であり、また BL07U には SPring-8 から移設された高効率の RIXS 装置がインストール準備中だったこともあり、参加者からの注目が高か

った。ビームラインやRIXS分光器を見ながら活発な議論が行われ、早期の実現を期待する声が多く、ワークショップの良い締めくくりができたと考えている。



図3 参加者の集合写真

#### 4. まとめ (Conclusion)

Workshop on Resonant Inelastic and Elastic X-ray Scattering を2023年8月2-4日に開催した。本ワークショップはシリーズとして開催されており、2018年までは対面形式で開催されていたが、2021年はオンライン形式であった。2023年は、5年ぶりに対面での開催が実現し、参加者間で活発な議論が交わされた。研究者間の交流は非常に有意義であり、特に NanoTerasu を軸として、東北大学金属材料研究所や量子科学技術研究開発機構との共同研究や技術連携に関して、新たな展開が生まれる転機になったと考えている。

#### 謝辞 (Acknowledgement)

本ワークショップに参加された講演者、聴講者の皆様に感謝します。本ワークショップは、東北大学金属材料研究所と量子科学技術研究開発機構次世代放射光施設整備開発センターの共同主催で開催しました。関係者の皆様に感謝いたします。また、GIMRT や前回主催のBNLからの支援に御礼申し上げます。



## Reimei-GIMRT Workshop Quantum Beams Study of the Dynamics of Rare Earth Garnets

August 7-8, 2023, IMR, Sendai

### Scope

The aim of the workshop was to explore the magnetism, dynamics, and transport properties of Rare-Earth Garnets in both bulk form and in films. The goal is to develop an adequate treatment of the complex magnetic dynamics which considers the non-collinear structures that appear in many of the compounds and their origin in terms of crystal field anisotropies acting on the rare-earth sites. The influence of the rare-earth moments on the chiral properties of the spin waves is of paramount importance in, for example, the spin Seebeck effect. Compensation points are potentially interesting for potential applications in spintronics as the magnetic dynamics are altered and domain wall motion enhanced. As well as bulk samples, it is now possible to study films, whose properties are directly relevant to device applications, and this raises issues about the influence of strain and other details of coupling to the lattice. Several groups internationally are looking at the dynamics by neutron inelastic scattering and, more recently, resonant magnetic X-ray scattering, and we hope to encourage discussion between them as to the interpretation of results that are currently being produced, and the availability of samples for future experiments.

### Program-Day 1

The morning session of day 1 started with opening address. The 1<sup>st</sup> scientific talk was on the synergetic investigation by polarized neutron and X-ray scattering for magnetic dynamics and the application to spin caloritronics by Dr. Mannix. Then Dr. Miyawaki introduced recent research on the X-ray scattering on quantum materials and the development of a soft-X-ray scattering station of NanoTerasu, which was in commissioning. The final talk in the morning was on the non-local magnon transconductance on the rare-earth magnetic garnet film by Dr. Kohno. The three talks highlight the different aspects of research on the system and show the importance of the collaboration among different techniques and views.

The afternoon session started with the talk of Dr. Geprägs on the magnonics, which is one of the

highlights of current spintronics research. The talk was followed by a report on neutron scattering by Dr. Peçanha-Antonio. Dr. Shamoto gave another talk combining neutron scattering under ultrasonic injection. These three talks show the interesting magnon properties of these systems.

The final session of Day 1 had two talks. The first was on magneto-crystalline anisotropy by Dr. Tomasello and the second on neutron scattering on the magnons of the terbium iron garnet, which has recently attracted much attention in magnonics and the cavity physics of magnons.

In the evening, participants had exchange and free discussion time.

### Program-Day 2

On day 2 the morning session began with mid-infrared spectroscopy on spintronics material by Dr. Puebla and Dr. Chudo gave a report on the Barnett effect and the observation of angular momentum.

Dr. Harii reported on the modification of magnetic properties of rare-earth magnetic garnet by ion beam irradiations. Dr. Nakamura talked about the ultrafast TEM measurement on the acoustically induced magnetic domains on ferromagnetic thin films.

The afternoon session started with the talk on the double umbrella structure by Dr. Thomas-Hunt. Dr. Omori show the combinatorial FMR experiments on magnetic garnet films. Dr. Hisatomi reported the Brillouin scattering experiment on yttrium magnetic garnet. The final talk was given by Dr. Hioki on the coherent dynamics on hybridized magnon-phonon.

Dr. Maekawa made a conclusion about the recent progress on rare-earth magnetic garnet shared in the workshop and future challenges for comprehensive collaboration research.

### Summary

The workshop offered an important opportunity for intense exchange among experts from different areas and succeeded in sharing of the current status of research. It is notable that many of the participants joined the X-ray scattering



# Workshops

workshop (RIXS and REXS) at the IMR, including a visit to NanoTerasu, and made visits to J-Parc for discussion on future collaborations. It shows the importance and the effectiveness of the GIMRT program to push the international collaborations.

## Name of organizers

Ieda Jun'ichi, ASRC, JAEA

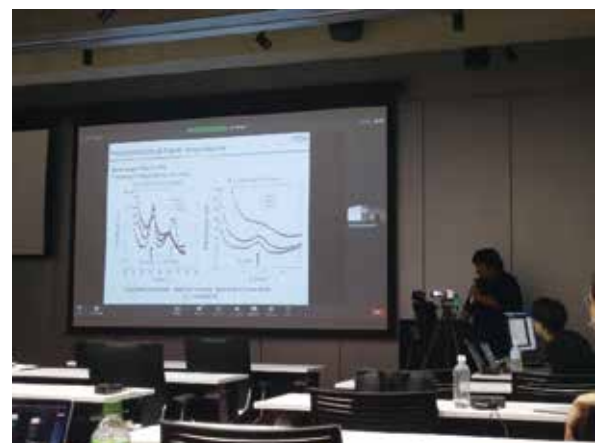
Mori Michiyasu, ASRC, JAEA

Fujita Masaki, IMR, Tohoku University

Nojiri Hiroyuki, IMR, Tohoku University

Ziman Timothy, ILL, Grenoble

Sakai Toru, University of Hyogo



## Program

|                  |                                       |                                                                                                                                        |
|------------------|---------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| Aug. 7 (Monday)  |                                       |                                                                                                                                        |
| 10:00            |                                       | Reception                                                                                                                              |
| 10:20            | K. Takanashi (JAEA)                   | Opening                                                                                                                                |
| 10:30            | D. Mannix (ESS)                       | Exploiting Polarised neutron and X-ray synergies to reveal magnetic structure and dynamics in spin caloritronics                       |
| 11:00            | J. Miyawaki (QST)                     | Quantum material research by resonant inelastic soft X-ray scattering facility at NanoTerasu                                           |
| 11:30            | R. Kohno (Tohoku)                     | Non-local magnon transconductance in extended rare-earth magnetic garnet films                                                         |
| 12:00            |                                       | Lunch                                                                                                                                  |
| 14:00            | S. Geprägs (Walther-Meißner-Institut) | Rare-earth iron garnets: A prototype material system for spintronics and magnonics                                                     |
| 14:30            | V. Peçanha-Antonio (U. Oxford)        | Rare earth iron garnets from the neutron scatter viewpoint                                                                             |
| 15:00            | S. Shamoto (CROSS)                    | Spin-lattice coupling in yttrium iron garnet studied by neutron scattering under ultrasound injection                                  |
| 15:30            |                                       | Break                                                                                                                                  |
| 16:00            | B. Tomasello (U. Kent)                | Role of magneto-crystalline anisotropies in complex rare-earth garnets                                                                 |
| 16:30            | Y. Kawamoto (IMR)                     | Neutron scattering studies for spin dynamics in terbium iron garnet                                                                    |
| 18:00            |                                       | Banquet                                                                                                                                |
| Aug. 8 (Tuesday) |                                       |                                                                                                                                        |
| 9:30             | J. Puebla (RIKEN)                     | Mid-infrared spectroscopy characterization of spintronic structures                                                                    |
| 10:00            | H. Chudo (JAEA)                       | Observation of the angular momentum compensation by using the Barnett effect                                                           |
| 10:30            |                                       | Break                                                                                                                                  |
| 11:00            | K. Harii (QST)                        | Modification of magnetic properties in garnets caused by swift ion beam irradiation                                                    |
| 11:30            | A. Nakamura (RIKEN)                   | Acoustically induced nonlocal magnetic domain dynamics in ferromagnet thin film revealed by ultrafast transmission electron microscopy |
| 12:00            |                                       | Lunch                                                                                                                                  |
| 14:00            | J. Thomas-Hunt (Aarhus)               | Renewed investigation of the double umbrella                                                                                           |
| 14:30            | Y. Omori (NEC)                        | Combinatorial experiments of FMR on magnetic garnet films                                                                              |
| 15:00            |                                       | Break                                                                                                                                  |
| 15:30            | R. Hisatomi (Kyoto)                   | Vorticity-inversion Brillouin light scattering by magnons in yttrium iron garnet crystal                                               |
| 16:00            | T. Hioki (U. Tokyo)                   | Coherent dynamics of hybridized magnons and phonons                                                                                    |
| 16:30            | S. Maekawa (RIKEN)                    | Closing                                                                                                                                |

## The 18th International Workshop on Biomaterials in Interface Science

研究代表者：東北大金研 加藤秀実

研究分担者：東北大歯学 金高弘恭 高橋信博 鈴木治 東北大医工学 西條芳文 成島尚之

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### 1. 概要

迫りくる高齢化社会において、医療への課題は多く、治療や診断などといった需要に関して、新規生体材料、医療機器の開発は求められている。例えば、人工骨や人工歯といった生体材料の開発には、ナノからマイクロスケールまでの幅広い機能や機械的特性の制御、人体との適合性など、さまざまな要求に応える必要がある。従って、限られた分野だけではなく、派生する異分野との共同、さらには、国際的な活動が必要とされる。そのため、本ワークショップは、2011年より生体材料研究を中心とし、材料分野、歯学分野、医工学分野の関係者が集まり開催されている。主な関係組織は、東北大学金属材料研究

所、歯学研究科、医工学研究科、さらに東京医科歯科大学生体材料工学研究所であり、それ

**Interface Summer Seminar 2023**

The 18th International Workshop on Biomaterials in Interface Science

**Invited Speaker:**

- Prof. Min Wang (The University of Hong Kong)
- Prof. Baek Il Kim (Yonsei University)
- Prof. Eun Hyun Park (Seoul National University)
- Prof. Gwyn Gould (University of Strathclyde)

Sponsored by Graduate School of Dentistry, Biomedical Engineering, Engineering, Institute for Materials Research, Tohoku University  
Tokyo Medical and Dental University  
Global Institute for Materials Research Tohoku (GIMRT)

**Date and Time** August 4, 2023 (Fri.) 9:00 – 17:00

**Hybrid Meeting (IMR and Online)**

**Topics**

- ① Oral Health Care
- ② Biomaterial
- ③ Biomedical Engineering
- ④ Young Investigators

**Online registration**

Please register by **July 31, 2023 (Mon.)**, Japan standard time

※ We will send the URL for participating in the seminar to all the applicants by the date of the seminar.  
※ Deadline for Abstract Submission: July 15 Sat., 2023

**URL** <https://forms.gle/Uf1JUQjsADAowWUG7>

**Contact:** Design Engineering by Joint Inverse Innovation for Material Architecture (DEJI<sup>2</sup>MA), Tohoku University  
Email: [rokkenpro-imr@grp.tohoku.ac.jp](mailto:rokkenpro-imr@grp.tohoku.ac.jp)



それぞれの組織が連携することにより、外国人研究者や学生などによる学際的な議論が行えるプラットフォームの提供を目指している。本ワークショップは、2023年8月4日に開催され、今回で18回目となりました。

## 2. 内容

東北大学金属材料研究所講堂を会場とし、オンラインとオンサイトを併用したハイブリット形式で開催しました。セッションテーマは①Biomaterials ②Oral Health Care ③Young innovators ④Biomedical Engineering の4つに分け、各セッション招待講演者1名、口頭発表者5名として実施しました。招待講演者4名のうち3名が来日し、香港大学の Min Wang 教授は“ Interfaces in Biomaterials and their Applications: Design, Control and Assessments”という研究題目で、韓国延世大学の Baek Il Kim 教授は“Optical detection of oral microbiome and its metabolites”という研究題目で、韓国ソウル大学の Eun Hyun Park 研究員は“A Novel Root Canal Irrigation System Utilizing Remotely Generated High-Power Ultrasound: Modes of Function, Cleaning Efficacy, and Safety”という研究題目で、それぞれ発表が行われました。英国ストラスクライド大学の Gwyn W. Gould 教授は、オンラインで参加し“Watching Fat cells: Studies of GLUT4 distribution using superresolution microscopy”という研究題目で発表が行われました。。参加者は82名（オンサイト44名、オンライン38名）であり若手研究者ならびに学生を中心に発表が繰り広げられました。対面での参加者が多く、長時間にわたる活発な議論が交わされるとともに、異分野間での交流がこなれました。



## 3. 謝辞

本ワークショップは、東北大学金属材料研究所 国際・産学連携インヴァースイノベーション材料創出プロジェクトが主催し、GIMRT の助成により実施されました。運営にご支援いただいたすべての方に謝意を表します。

# The 6th Symposium for the Core Research Clusters for Materials Science and Spintronics, and the 5th Symposium on International Joint Graduate

## Program in Materials Science

研究代表者：東北大学金研 折茂慎一<sup>1</sup>

研究分担者：東北大学材料科学コアリサーチクラスター / AIMR 貞許礼子<sup>2</sup>

Shin-ichi Orimo<sup>1</sup>, Reiko Sadamoto<sup>2</sup>

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Keywords: materials science, core research cluster, international joint graduate program

Tohoku University was named one of the first three Designated National Universities in Japan on June 30, 2017 by the Japanese Government. As a Designated National University, we initiated the “Core Research Clusters” to strengthen four research fields: materials science, spintronics, next-generation medical care and disaster science. Also, International Joint Graduate Program in Materials Science aims to cultivate internationally capable and highly creative professionals in the materials science field. In order to present research activities and discuss future prospects, we hold, continuing from past years, the international symposium on the Materials Science and Spintronics on November 18 – December 1, 2023.

### 1. 緒言

東北大学は、2017年6月30日、日本で最初の3つの指定国立大学の一つに選ばれた。指定国立大学の事業として、東北大学が強みを有する材料科学、スピントロニクス、未来型医療、災害科学の4つの研究分野を世界トップレベル研究拠点として整備し研究推進している。また、材料科学研究分野では国際的に活躍できる創造性豊かな人材を育成することを目的とした「材料科学国際共同大学院プログラム」(GP-MS)を実施している。この材料科学世界トップレベル研究拠点(CRC-MS)、スピントロニクス世界トップレベル研究拠点(CSIS)および材料科学とスピントロニクスそれぞれの大学院プログラム(GP-MSおよびGP-Spin)の活動と研究成果を発表し、今後の展望を議論するために、2023年11月28–12月1日に第7回目となる国際シンポジウムを対面形式(一部はハイブリッド形式)にて開催した。なお、2022年のシンポジウムに引き続き今回も本学の世界トップレベル研究拠点の目標の1つである学内の卓越したリソースの結集の一環として、各拠点やセンター、プログラム等の構成部局に加えて、金属材料研究所国際共同利用・共同研究拠点(GIMRT)も共催として合同で開催した。

### 2. 開催内容

第7回目となる本国際シンポジウムでは、CRC-MS 点に設置された4領域の企画セッションのほか、CSIS によ





るセッション、第6回目となる GP-MS に参画する大学院生による企画セッション、GP-Spin によるセッションが、片平さくらホール、AIMR セミナールーム、ナノスピ棟カンファレンスルームの3会場を使用して行われた。前回はオンライン中心のハイブリッドであったが、今回は対面開催を中心として、一部（プレナリー講演など）はハイブリッドで開催した。4日間の会期中に4件のプレナリー講演（うち2名が外国人）のほか、国内外および学内からの招待講演により、CRC-MS では4セッション14名、GP-MS では6セッション19名、CSIS では7セッション16名、GP-Spin では2セッション8名の合計19セッション57名の口頭発表が行われた。また、シンポジウム1日目に CRC-MS Award 受賞者2名および CRC-Spin Award 受賞者2名による受賞講演を行い、夕刻のレセプションにて授賞式を執り行い、受賞した4名の若手研究者の研究を世界へ発信する機会とした。シンポジウムのポスターセッションでは、91件の発表があり、審査により10件のベストポスター賞が選ばれ、4日目に授賞式が行われた。

- ・参加者：合計301名（日本：266名、海外：35名）

#### 【セッション概要】

##### (1)Plenary セッション

- ・Plenary 講演：4セッションー海外2名

##### (2)Invited セッション

- ・CRC-MS：4セッション14名ー学内4名、学外10名（うち海外8名）
- ・GP-MS：6セッション19名ー学内6名、学外13名（うち海外13名）
- ・CSIS（CRC-Spin）：7セッション16名ー学内3名、学外13名（うち海外10名）
- ・GP-Spin：2セッション8名ー学内0名、学外8名（うち海外4名）

##### (3)Poster セッション

- ・91件

#### ● 1日目（2023年11月28日）

まず、大野英男東北大学総長の開会挨拶ビデオメッセージに引き続き、CRC-MS 副拠点長（折茂）の司会により、小田玲子ボルドー大学教授/東北大学プロフェッサー、ユニバーシティ・リサーチ・リードによる”Transferring Chiral Information between Objects with different dimensions without crystalline order”、佐々木孝彦教授を座長として Henning Sirringhaus ケンブリッジ大学教授による”Transient localization and spin relaxation physics of high mobility organic semiconductors”の2件のプレナリー講演が行われた。午後には、ポスターセッション1に引き続き、3件めのプレナリー講演 Di-Jing Huang 台湾国立清華大学教授による”Spin and Charge Excitations of Unconventional Superconductors Probed by High-Resolution RIXS”が組頭広志教授を座長として行なわれた。次に、CRC-MS Award 2024 および CRC-Spin Award 2024 の受賞者による受賞講演、ポスターセッション2が行われた。ポスター発表は昨年とは違い対面形式のみの開催であり、活発な討論が行われた。

- ・ポスター発表数：91件（材料科学分野46件、スピントロニクス分野41件）
- ・ポスター発表表彰：Best Poster Award 10件

午後6時からウェスティンホテルにてレセプションパーティが大野英男東北大学総長による開宴挨拶・乾杯で始まり、小谷元子理事研究担当理事・シンポジウム大会長の閉宴挨拶で終了した。レセプションパーティの時間を活用して CRC-MS Award および CRC-Spin Award 受賞者への賞状・盾の授与が行われた。

#### ● 2日目（2023年11月29日）

午前中に CRC-MS のセッション2件と GP-MS セッション1件が、午後には CRC-MS のセッション1件、GP-MS の学生セッション2件、GP-Spin のセッション1件が開催された。

#### ● 3日目（2023年11月30日）

午前中に CRC-MS のセッション1件と GP-MS セッション1件、GP-Spin セッション1件が開催された。午後には、プレナリー講演4件目、中辻知東京大学教授による”Topological Magnetic Materials for Innovative Quantum

Electronics”が深見俊輔教授を座長として開催されたほか、GP-MS の学生セッション 1 件、CSIS (CRC-Spin) のセッション 3 件が開催された。

- 4 日目 (2023 年 12 月 1 日)

最終日は、午前中に CRC-MS セッション 1 件、GP-MS の学生セッション 1 件、CSIS (CRC-Spin) のセッション 2 件が行われた。午後は CSIS (CRC-Spin) のセッション 2 件が開催されたのち、ベストポスター賞の発表および賞状授与式が行われ、シンポジウム実行委員長 (折茂) による closing remarks により終了した。

### 3. まとめ

第 7 回となる本シンポジウムでは、対面開催を中心とすることにより (一部はハイブリッド開催)、多くの研究者がつどい情報交換をする場を提供することができた。本学の材料科学分野およびスピントロニクス分野に関する多くの部局・拠点・プログラム等の参画により、また、本学の研究者の発表もこれまで以上にプログラムに盛り込まれていたこともあり、本学の優れた研究成果を国内外により広くアピールすることができた。次回以降の国際シンポジウム開催に向けて、本学の研究力発信と研究力向上にさらに貢献できるように準備を進めていく予定である。

### 謝辞

本シンポジウムは、材料科学世界トップレベル研究拠点(CRC-MS)、スピントロニクス世界トップレベル研究拠点(CSIS)、材料科学国際共同大学院プログラム(GP-MS)、スピントロニクス国際共同大学院プログラム(GP-Spin)、が共同主催し、東北大学高等研究機構 International Affairs Center(IAC)の協力のもと GIMRT の共催により実施されたものです。また、助成いただいた新技術振興渡辺記念会および仙台国際観光協会と、運営・企画に参画されたすべての方に謝意を表します。

### 引用文献 (Reference)

1) シンポジウムホームページ

[https://www.crc-ms.tohoku.ac.jp/en/news/2023/11/Symposium2023\\_index.html](https://www.crc-ms.tohoku.ac.jp/en/news/2023/11/Symposium2023_index.html)

2) ベストポスター賞受賞者掲載ページ

[https://www.crc-ms.tohoku.ac.jp/en/news/2023/11/Symposium2023\\_Bestposter\\_index.html](https://www.crc-ms.tohoku.ac.jp/en/news/2023/11/Symposium2023_Bestposter_index.html)

3) シンポジウムタイムテーブル

[https://www.crc-ms.tohoku.ac.jp/en/news/2023/11/symposium2023\\_timetable.pdf](https://www.crc-ms.tohoku.ac.jp/en/news/2023/11/symposium2023_timetable.pdf)

**The 7th Symposium for the Core Research Clusters for Materials Science and Spintronics and  
the 6th Symposium on International Joint Graduate Program in Materials Science and Spintronics**

**Timetable 1 (November 28 - 29)**

| November 28(Tue)                           |                                  |                                 | November 29(Wed)                           |                                                                  |                                                 |
|--------------------------------------------|----------------------------------|---------------------------------|--------------------------------------------|------------------------------------------------------------------|-------------------------------------------------|
| Location                                   |                                  |                                 |                                            |                                                                  |                                                 |
| Sakura Hall                                | AIMR Main Bld<br>2F Seminar room | Nano Spin 4F<br>Conference room | Sakura Hall                                | AIMR Main Bld<br>2F Seminar room                                 | Nano Spin 4F<br>Conference room                 |
|                                            |                                  |                                 | 9:00- CRCMS1                               |                                                                  |                                                 |
| 9:40- Opening                              |                                  |                                 | Advances in soft<br>materials<br>(CM1-1~3) |                                                                  |                                                 |
| 9:45- Plenary1<br>(Reiko Oda)              |                                  |                                 |                                            | 10:00- GP-MS1                                                    |                                                 |
| 10:30- Plenary 2<br>(Henning Sirringhaus)  |                                  |                                 |                                            | Student Session 1<br>Oxide electronics<br>(GM1-1~3)              |                                                 |
|                                            | Break                            |                                 |                                            |                                                                  |                                                 |
| 11:30- Photo                               |                                  |                                 |                                            |                                                                  |                                                 |
|                                            | 12:00- Lunch Time                |                                 |                                            | 12:00- Lunch Time                                                |                                                 |
| 13:30-<br>Poster Session1                  |                                  |                                 |                                            | 13:30- GP-MS2                                                    | 13:30- CRCMS2                                   |
| 14:15- Plenary3<br>(Di-jing Huang)         |                                  |                                 |                                            | Student Session 2<br>Porous materials<br>(GM2-1~3)               | Quantum materials<br>and magnonics<br>(CM2-1~3) |
|                                            | Break                            |                                 |                                            |                                                                  | Break                                           |
| 15:15-<br>CRC Award talk                   |                                  |                                 |                                            | Break                                                            | 15:15- GP-Spin1                                 |
|                                            | Break                            |                                 |                                            | 16:00- GP-MS3                                                    | Spin-functional<br>materials<br>(GS1-1~4)       |
| 16:15-<br>Poster Session2                  |                                  |                                 |                                            | Student Session 3<br>Energy conversion &<br>storage<br>(GM3-1~3) |                                                 |
|                                            |                                  |                                 |                                            |                                                                  |                                                 |
| 18:00- Symposium Reception (Westin Sendai) |                                  |                                 |                                            |                                                                  |                                                 |

The 7th Symposium for the Core Research Clusters for Materials Science and Spintronics and  
the 6th Symposium on International Joint Graduate Program in Materials Science and Spintronics

Timetable 2 (November 30 - December 1)

| November 30(Thu)                                |                                                                              |                                               | December 1(Fri)                                                               |                                  |                                                                                   |                                               |
|-------------------------------------------------|------------------------------------------------------------------------------|-----------------------------------------------|-------------------------------------------------------------------------------|----------------------------------|-----------------------------------------------------------------------------------|-----------------------------------------------|
| Location                                        |                                                                              |                                               |                                                                               |                                  |                                                                                   |                                               |
| Sakura Hall                                     | AIMR Main Bld<br>2F Seminar room                                             | Nano Spin 4F<br>Conference room               | Sakura Hall                                                                   | AIMR Main Bld<br>2F Seminar room | Nano Spin 4F<br>Conference room                                                   |                                               |
|                                                 |                                                                              |                                               |                                                                               |                                  |                                                                                   |                                               |
| 9:00- CRCMS3                                    |                                                                              | 9:00- GP-Spin2                                | 9:00- CRCMS4                                                                  |                                  | 9:00- CRCS4                                                                       |                                               |
| Multi-material design<br>& control<br>(CM3-1~5) | 10:00- GP-MS4                                                                | Spintronics devices<br>(GS2-1~4)              | Advanced carbon-<br>based materials for<br>batteries and sensors<br>(CM4-1~3) | 10:00- GP-MS6                    | Invited talk<br>(CS4-1~3)                                                         |                                               |
|                                                 | Student Session 4<br>Thermoelectric<br>materials<br>(GM4-1~3)                |                                               |                                                                               |                                  | Break                                                                             |                                               |
|                                                 |                                                                              |                                               | Break                                                                         |                                  | Student Session 6<br>Interface science and<br>engineering of joining<br>(GM6-1~3) | 10:50- CRCS5<br><br>Invited talk<br>(CS5-1~2) |
| 12:00- Photo                                    |                                                                              |                                               |                                                                               | 12:00- Lunch Time                |                                                                                   |                                               |
|                                                 | 12:30- Lunch Time                                                            |                                               |                                                                               |                                  |                                                                                   |                                               |
|                                                 |                                                                              | 13:25- Opening(Spin)                          |                                                                               |                                  |                                                                                   |                                               |
|                                                 |                                                                              | 13:30- Plenary4<br>(Satoru Nakatsuji)         |                                                                               |                                  | 13:30- CRCS6<br><br>Invited talk<br>(CS6-1~2)                                     |                                               |
|                                                 |                                                                              | 14:15- CRCS1<br><br>Invited talk<br>(CS1-1~2) |                                                                               |                                  | Break                                                                             |                                               |
|                                                 |                                                                              | Break                                         |                                                                               |                                  | 14:50- CRCS7<br><br>Invited talk<br>(CS7-1~2)                                     |                                               |
|                                                 | 15:30- GP-MS5                                                                | 15:35- CRCS2                                  |                                                                               |                                  | 15:50- Closing (Spin)                                                             |                                               |
|                                                 | Student Session 5<br>Theoretical<br>condensed matter<br>physics<br>(GM5-1~4) | Invited talk<br>(CS2-1~3)                     |                                                                               |                                  |                                                                                   |                                               |
|                                                 |                                                                              | Break                                         |                                                                               |                                  | 16:30-<br>Poster Award                                                            |                                               |
|                                                 |                                                                              | 17:20- CRCS3                                  |                                                                               |                                  | 17:00- Closing                                                                    |                                               |
|                                                 |                                                                              |                                               |                                                                               |                                  | Invited talk<br>(CS3-1~2)                                                         |                                               |
|                                                 |                                                                              |                                               |                                                                               |                                  |                                                                                   |                                               |
|                                                 |                                                                              | 19:00-<br>Banquet (Spin only)                 |                                                                               |                                  |                                                                                   |                                               |



# KINKEN WAKATE 2023: International Materials Science School 2023-Advances in Strongly Correlated Electron Systems

## Joint workshop: Topology, spin-orbit interactions and superconductivity in strongly correlated quantum materials under extreme conditions

Dai Aoki

IMR, Tohoku University, Oarai, Ibaraki 311-1313

Keywords: spin-orbit coupling, hidden order, UTe<sub>2</sub>, superconductivity, Fermi surface

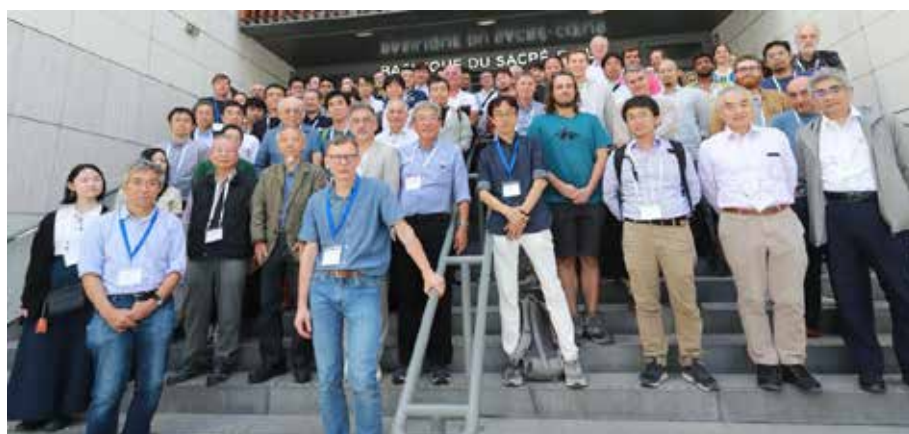
The International Materials Science School 2023 (KINKEN WAKATE 2023) took place on October 9, 2023, in Grenoble, France. This event was followed by the international workshop titled “Topology, Spin-Orbit Interactions, and Superconductivity in Strongly Correlated Quantum Materials under Extreme Conditions” from October 10 to October 12, 2023, making it a joint event.

The school and the workshop aimed to discuss and exchange recent progress in the study of strongly correlated quantum materials under extreme conditions such as high fields, high pressure, and low temperatures. These conditions are critical for understanding phenomena like topological effects, spin-orbit interactions, superconductivity, multiple orders, and fermiology. On the first day, the school was held at the high-field laboratory in Grenoble (LNCMI-G). It featured two tutorial lectures by Prof. Yoichi Yanase and Prof. Rikio Settai. Prof. Yanase discussed topological superconductivity, while Prof. Settai focused on quantum oscillation effects. In addition to the lectures, participants had the opportunity to tour the high-field lab and attend short poster previews.

From the second to the fourth day, the international workshop took place at the Basilique du Sacré-Cœur, located near the Grenoble train station. The workshop included a total of 36 oral presentations and 21 poster presentations. Researchers and students from around the world gathered to share their findings and discuss various topics related to quantum materials.

The workshop provided an excellent platform for the exchange of ideas and the establishment of collaborations. The diverse range of presentations covered cutting-edge research in topological phenomena, the interplay between spin-orbit interactions and superconductivity, and the physical properties under extreme conditions. This event highlighted the importance of multidisciplinary approaches in advancing our understanding of strongly correlated quantum materials.

Overall, the International Materials Science School 2023 and the subsequent workshop were successful in fostering discussions and collaborations among researchers and students, contributing significantly to the field of quantum materials science.





|         |       |                             | Basilique du Sacre-Coeur |       |                |                  |      |       |       |                   |       |                  |       |                  |            |                   |  |
|---------|-------|-----------------------------|--------------------------|-------|----------------|------------------|------|-------|-------|-------------------|-------|------------------|-------|------------------|------------|-------------------|--|
|         |       |                             | Time                     |       | 10 Oct. (Tue.) |                  | Time |       |       | 11 Oct. (Wed.)    |       | Time             |       | 12 Oct. (Thu.)   |            |                   |  |
| LNCMI-G |       |                             | 8:30                     | 8:50  | Registration   |                  |      |       |       |                   |       |                  | 8:30  | 9:00             | Hasselbach |                   |  |
|         |       |                             | 8:50                     | 9:00  | Opening        |                  |      |       |       | 8:30              | 9:00  | Behnia           |       | 8:30             | 9:00       | Hasselbach        |  |
|         |       |                             | 9:00                     | 9:30  | Harima         |                  |      |       |       | 9:00              | 9:30  | Izawa            |       | 9:00             | 9:30       | Kambe             |  |
|         |       |                             | 9:30                     | 10:00 | Onuki          |                  |      |       |       | 9:30              | 10:00 | Kotegawa         |       | 9:30             | 10:00      | Tou               |  |
|         |       |                             | 10:00                    | 10:30 | Araki          |                  |      |       |       | 10:00             | 10:30 | Suzuki           |       | 10:00            | 10:30      | Julien            |  |
|         |       |                             | 10:30                    | 11:00 | Break          |                  |      |       |       | 10:30             | 11:00 | Poster I & Break |       | 10:30            | 11:00      | Poster II & Break |  |
|         |       |                             | 11:00                    | 11:30 | de Visser      |                  |      |       |       | 11:00             | 11:30 | Hassinger        |       | 11:00            | 11:30      | Measson           |  |
|         |       |                             | 11:30                    | 12:00 | Spalek         |                  |      |       |       | 11:30             | 12:00 | K. Miyake        |       | 11:30            | 12:00      | Shishido          |  |
|         |       |                             | 12:00                    | 12:30 | Suderow        |                  |      |       |       | 12:00             | 12:30 | Amitsuka         |       | 12:00            | 12:30      | Watanabe          |  |
|         |       |                             | 12:00                    | 14:00 | Lunch          |                  |      |       |       | 12:00             | 14:00 | Lunch            |       | 12:00            | 14:00      | Lunch             |  |
| Time    |       | 9 Oct. (Mon.)               |                          |       |                |                  |      |       |       |                   |       |                  |       |                  |            |                   |  |
| 14:00   | 15:15 | Yanase (tutorial)           |                          | 14:00 | 14:30          | Bauer            |      | 14:00 | 14:30 | Ishida            |       | 14:00            | 14:30 | Penc             |            |                   |  |
|         |       |                             |                          | 14:30 | 15:00          | Onimaru          |      | 14:30 | 15:00 | Knafo             |       | 14:30            | 14:45 | Garbarino        |            |                   |  |
| 15:15   | 16:15 | Break & High-Field Lab Tour |                          | 15:00 | 15:30          | Utsumi Boucher   |      | 15:00 | 15:30 | A. Miyake         |       | 14:45            | 15:15 | Raymond          |            |                   |  |
|         |       |                             |                          | 15:30 | 16:00          | Poster I & Break |      | 15:30 | 16:00 | Poster II & Break |       | 15:15            | 15:45 | Flouquet         |            |                   |  |
| 16:15   | 16:45 | Short Poster Preview        |                          | 16:00 | 16:30          | Ohara            |      | 16:00 | 16:30 | Yanagisawa        |       | 15:45            | 16:00 | Closing (Harima) |            |                   |  |
| 16:45   | 18:00 | Settai (tutorial)           |                          | 16:30 | 17:00          | Matsuda          |      | 16:30 | 17:00 | Kimata            |       |                  |       |                  |            |                   |  |
|         |       |                             |                          | 17:00 | 17:30          | Pourret          |      | 17:00 | 17:30 | Fujimoto          |       |                  |       |                  |            |                   |  |
|         |       |                             |                          |       |                |                  |      | 19:00 |       | Workshop Dinner   |       |                  |       |                  |            |                   |  |

## KINKEN WAKATE 2023に参加した学生の会議報告

材料科学若手学校（KINKEN WAKATE 2023）と国際ワークショップ "Workshop on Topology, Spin-Orbit Interactions and Superconductivity in Strongly Correlated Quantum Materials under Extreme Conditions" (H-Physics Workshop) が、2023年10月9日から12日までグルノーブルで開催されました。参加者は合計78名で、37件の口頭発表と22件のポスター発表が行われました。学生の参加者は13名でした。日本から参加した学生のうち、以下の6名については、ICC-IMRと学術変革「アシンメトリ量子」から旅費が補助されました。A4半分程度の英語での会議報告を求めた結果、以下の通り会議報告がありました。

会議期間中には、ILL、LNCMI、ESRF、Institute Neel、CEAなどの大型研究施設やグルノーブルの主要な研究室を訪問した学生もいて、大変刺激を受けたようです。また、フランスの学生との交流や、会議中のポスター発表でのディスカッションも大変有意義だったとのこと。このように、若手が海外で交流する機会を設けることは、将来を担う若手育成という意味で非常に意義深いものです。ICC-IMRからの支援にあらためて感謝いたします。

青木 大

## Report on H-Physics workshop

Fusako KON

Hokkaido University

This report documents my participation in “H-Physics workshop” held in Grenoble France, from October 9 to 12. On the first day, I attended the tutorial session. The presentations are given by Prof. Yanase and Prof. Settai. Each provided a comprehensive overview of the historical background and recent results in the field of strongly correlated electron systems from the perspectives of theoretical studies of unconventional superconductivity and experimental studies using dHvA effects, respectively.

From the second day to the final days, many oral presentations are given by researchers from several countries. These presentations covered a wide range of materials, including attractive unconventional superconductors such as  $\text{UTe}_2$  and  $\text{CeRh}_2\text{As}_2$ , as well as other strongly correlated f-electron and d-electron systems, and even quasicrystal systems. In addition to the oral sessions, we had poster sessions. In the poster sessions, I presented my recent studies on  $\text{UPt}_2\text{Si}_2$  and discussed with some participants. This allowed me to gain diverse insights into my research.

The participants shared not only their results but also some episodes about their research lives. These episodes showed how the international collaborations and the cooperations between theoretical and experimental researchers can develop new research possibilities. In fact, I got the opportunity to establish international personal connections through the workshop, and the interactions with female researchers actively working abroad were particularly inspiring and encouraging for me.

I am grateful for these experiences and will apply them to my future research activities.

Taiki Miyamoto  
Osaka University

I participated in the workshop in Grenoble and went to laboratory tour in CEA, ILL, ESRF and CNRF. I will report about these activities.

In the workshop, I presented our research in a poster section. Our research about a magnetic toroidal system is not well-known foreign countries, and actually, many researchers didn't know the magnetic toroidal multipole and the concept of cluster multipole. Therefore, I had to explain not only brief background but also more basic and detail background. For me, it was very difficult to explain that in English. This opportunity is very valuable for me because I have never participated in international conference.

In laboratory tour, I went to CEA, ILL, ESRF, and CNRF. I haven't been to large laboratory, so I was surprised that all buildings are optimized for experiments. For example, in CEA, all pumps are placed in rooms dedicated to pumps, and vibrations from pumps to probes are completely eliminated. I was most interested in scanning SQUID in Prof. Klaus Hasselbach's laboratory. His SQUID tip was nano-SQUID, and the tip also has a needle for AFM. To make nano-SQUID, high sensitivity photolithography is needed and the laboratory, of course, has it. By having AFM with SQUID tip, the scan becomes more accurate. One of the things which realize such a scan is the building. The building eliminates a vibration from the ground. In our laboratory, we couldn't do this experiment due to vibration.

In conclusion, this experience is very valuable for my future. I will be willing to participating in like this opportunity in the future. Thank you very much for your great support.

## Report of H-Physics workshop in 10/9~10/12 @Grenoble, France

Ryohei Oishi, Hiroshima University

Supported by ICC-IMR, I visited Grenoble, France to attend a H-Physics workshop in 10/9~10/12. Many kinds of research of condensed matter, for example Fermi Surface, U-based compounds, and multipoles etc, were given lectures in the workshop. My purpose of visit is to discuss our works of  $RPt_6Al_3$  and to find Postdoc jobs after finishing a PhD course.

For the Dr. E. Bauer's talk about "Yb compounds: a rich playground for unconventional ground states", he discussed about the frustrated Kondo lattice compounds. I could get the opportunity to discuss our result of honeycomb Kondo lattice compound  $CePt_6Al_3$  with him, which gave us one idea to distinguish the role of Kondo effect and frustration. In my poster presentation for 30 + 30 min, I discussed about the geometrical condition induces DM interaction in  $RPt_6Al_3$  with centrosymmetric structure. Finally, every researcher agreed with our idea.

We visited CEA, ILL, ESRF, and CNRS before workshop. Because I would like to find a Postdoc job of synthesizing single crystals by a variety of methods, I was so excited to see the equipment of crystal growth and talk with Dr. Gerard in CEA. For synthesizing crystals by Czochralski method, Dr. Gerard designed a holder of seed crystal, which can arrange the position by himself. These original technics surprised me, and I plan to design myself in Japan.



## Report of H-Physics workshop @ Grenoble, France

Kenta Sudo (IMR, Tohoku Univ., Japan)

I attended the tutorial session "Kinken-Wakate 2023" on "Topology, spin-orbit interactions and superconductivity in strongly correlated quantum materials under extreme conditions" in Grenoble, France, held on 2023/10/09. Here, I performed short poster preview that is summary of my poster will be talked in main session.

Main session of H-physics work shop was held on 10/10-10/12. In the main session, I performed poster presentation "Spontaneous nonreciprocal resistance in a zig-zag antiferromagnet NdRu<sub>2</sub>Al<sub>10</sub>". Then I had discussions with the participants and deepened my consideration of my research results. Furthermore, I attended all lecture and got new idea for my next research.

Finally, I visited the Neel Institute in Grenoble, France, and had discussions with Klaus Hasselbach and Arnaud Badel. As a result, I got new ideas to develop my own research topic. In addition, I succeeded making global research network.

## The report of H-physics workshop

Hiroto Suzuki, Hiroshima University

I went to Grenoble to participate in the H-physics workshop and to visit some laboratories from October 3 to 16. The visit allowed us to go to CEA, ILL, ESRF, and CNRS. I was impressed by the research-first approach taken throughout the building design. Specifically, a room existed just for the installation of refrigeration pumps to avoid noise and vibration. In addition, I was surprised that there is a technician just for the synthesizing crystal. This visit to an overseas laboratory was the first time for me. These laboratories have many different things with Japanese laboratories. This experience broadened my mind.

At the Workshop, I gave a poster presentation on my discovery of a new material titled “Anisotropic antiferromagnetic order in orthorhombic  $\text{EuPdAl}_6$ ”. Not only Japanese but also French students listened to and were interested in my presentation. I could discuss it with them. After the tutorial workshop, Co-chairs arranged for us to have the opportunity to meet with French students. They took us to a bar in Grenoble and I was able to deepen my friendship with them. Throughout the workshop and visiting laboratories, I realized my lack of English skills. In the future, I would like to make more efforts in both research and English and I can make better presentations at international conferences.

## Report of H-Physics Workshop

|                 |                                                                                                                           |      |                  |
|-----------------|---------------------------------------------------------------------------------------------------------------------------|------|------------------|
|                 |                                                                                                                           | Name | Hiroki Matsumura |
| Conference name | Topology, spin-orbit interactions and superconductivity in strongly correlated quantum materials under extreme conditions |      |                  |
| Place           | Grenoble, France                                                                                                          |      |                  |
| Date            | 2023/10/9 – 2023/10/12                                                                                                    |      |                  |

With the support of ICC-IMR, I participated in the H-Physics Workshop held in Grenoble, France.

This is an international workshop to discuss the results of research on strongly correlated electron systems under extreme conditions. The meeting was a very useful opportunity to learn about cutting-edge research results, both theoretical and experimental studies.

I gave a poster presentation on the recent progress of NMR measurements on the spin-triplet superconductor  $\text{UTe}_2$ , and was able to discuss the results with many researchers.

Finally, I would like to acknowledge ICC-IMR for financially supporting me and Prof. Aoki and other co-chairs for providing me with this valuable opportunity.

## Summit of Materials Science SMS 2023 and Global Institute for Materials Research Tohoku (GIMRT) User Meeting 2023 , November 20-22, 2023



The 6th SMS was successfully held at IMR auditorium with almost 200 of participants (including online participants) in 3 days from November 20 to 22. All speakers gathered in a hall after an interval of four years since the last onsite meeting of 4th SMS held just before the pandemic.



The Conference started with the welcome greetings by Prof. Takahiko Sasaki, Director of IMR, Prof. Hideo Ohno, President of Tohoku University and Mr. Koji Yanagisawa, Director of Scientific Research Institutes Division, MEXT (Ministry of Education, Culture, Sports, Science and Technology). The auditorium was fulfilled with over a hundred of participants from all over the world.

The conference was divided in 9 fields, "Superconductivity", "Quantum Materials", "Exotic Spin Systems", "Material Design and Informatics", "Spintronics and Topological Phenomena", "Functional Materials", "Nuclear and Irradiation", "Advanced Metallurgy – 3D Printing and Nanomaterials" and "Hydrogen Materials". A hot discussion was exchanged at every field, and a discussion sometimes extended for a break. In the evening of 2nd day, the poster session was held. Researchers and students presented their recent research topics. The discussion was overflowing with excitement and enthusiasm and continued until late at night.

The total number of speakers were 48 this time. 20 were invited, in which 11 were from overseas, and 28 were contributed or short speakers. Not only senior researchers, but also young and energetic speakers expressed lively their recent cutting-edge research topics.



# Summit of Materials Science 2023 and GIMRT User Meeting 2023

Date: November 20-22, 2023

Venue: IMR Auditorium, Tohoku University, Onsite, hybrid available

MAP: [https://www.tohoku.ac.jp/en/about/images/map\\_katahira\\_2021.pdf](https://www.tohoku.ac.jp/en/about/images/map_katahira_2021.pdf)

## Day 1: Nov. 20

|  | 10:00 | 10:20 | Opening (Chair: Rie Y. Umetsu, IMR) |                 |                                                                                      |  |
|--|-------|-------|-------------------------------------|-----------------|--------------------------------------------------------------------------------------|--|
|  |       |       | Opening Address                     | Takahiko Sasaki | Director of Institute for Materials Research, Tohoku University                      |  |
|  |       |       | Welcome Greeting                    | Hideo Ohno      | President of Tohoku University                                                       |  |
|  |       |       | Greeting from MEXT                  | Koji Yanagisawa | Director of Scientific Research Institutes Division, Research Promotion Bureau, MEXT |  |

| Number                                                      | Time  | Category | Name        | Affiliation       | Title                           | Page                                                                                                                                                                                                |    |
|-------------------------------------------------------------|-------|----------|-------------|-------------------|---------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Session A Superconductivity (Chair: Masaki Fujita, IMR)     |       |          |             |                   |                                 |                                                                                                                                                                                                     |    |
| <a href="#">A-1</a>                                         | 10:20 | 10:50    | Invited     | Youichi Yanase    | Kyoto University                | Diverse mechanism of spin-triplet superconductivity                                                                                                                                                 | 7  |
| <a href="#">A-2</a>                                         | 10:50 | 11:20    | Invited     | Clifford W. Hicks | University of Birmingham        | Stress-strain measurements of the unconventional superconductor Sr <sub>2</sub> RuO <sub>4</sub>                                                                                                    | 8  |
| <a href="#">A-3</a>                                         | 11:20 | 11:40    | Contributed | Dai Aoki          | IMR                             | Multiple superconducting phases and Fermi surfaces in spin-triplet superconductor UTe <sub>2</sub>                                                                                                  | 9  |
| <a href="#">A-4</a>                                         | 11:40 | 12:00    | Contributed | Tsutomu Nojima    | IMR                             | Nonreciprocal Superconducting Transport with Ferroelectric Polarization in Ion-Gated SrTiO <sub>3</sub>                                                                                             | 10 |
| <a href="#">A-5</a>                                         | 12:00 | 12:20    | Contributed | Motoki Osada      | IMR                             | Optimizing synthesis of superconducting infinite-layer nickelate thin films                                                                                                                         | 11 |
|                                                             | 12:20 | 13:30    | Lunch       |                   |                                 |                                                                                                                                                                                                     |    |
| Session B Quantum Materials (Chair: Dai Aoki, IMR)          |       |          |             |                   |                                 |                                                                                                                                                                                                     |    |
| <a href="#">B-1</a>                                         | 13:30 | 14:00    | Invited     | Emilia Morosan    | Rice University                 | Real- and reciprocal-space topology in the square net series Eu(Ga <sub>1-x</sub> Al <sub>x</sub> ) <sub>4</sub>                                                                                    | 13 |
| <a href="#">B-2</a>                                         | 14:00 | 14:30    | Invited     | Shintaro Ishiwata | Osaka University                | Exploration of metastable perovskite oxides exhibiting exotic magnetism: Combination of high-pressure synthesis and structural prediction                                                           | 14 |
| <a href="#">B-3</a>                                         | 14:30 | 15:00    | Invited     | Valentin Taufour  | University of California, Davis | Combining Topology and Superconductivity: Can We Discover Unconventional Superconductors Methodically?                                                                                              | 15 |
| <a href="#">B-4</a>                                         | 15:00 | 15:20    | Contributed | Michi-To Suzuki   | IMR                             | Exploring Functional Antiferromagnetic Materials with Magnetic Structure Screening and First-Principles Calculation                                                                                 | 16 |
| <a href="#">B-5</a>                                         | 15:20 | 15:40    | Contributed | Wataru Kosaka     | IMR                             | Creation of Gas-Responsive Porous Magnet                                                                                                                                                            | 17 |
|                                                             | 15:40 | 15:55    | Break       |                   |                                 |                                                                                                                                                                                                     |    |
| Session C Exotic Spin Systems (Chair: Hiroyuki Nojiri, IMR) |       |          |             |                   |                                 |                                                                                                                                                                                                     |    |
| <a href="#">C-1</a>                                         | 15:55 | 16:25    | Invited     | Kwang-Yong Choi   | Sungkyunkwan University         | Ground state and spin dynamics of the Kagome antiferromagnet YCu <sub>3</sub> (OD) <sub>6+x</sub> Br <sub>3-x</sub>                                                                                 | 19 |
| <a href="#">C-2</a>                                         | 16:25 | 16:55    | Invited     | Bella Lake        | Helmholtz-Zentrum Berlin        | Quantum spin liquid behavior and ferroelectricity in PbCuTe <sub>2</sub> O <sub>6</sub>                                                                                                             | 20 |
| <a href="#">C-3</a>                                         | 16:55 | 17:25    | Invited     | Masato Matsuura   | CROSS*                          | Lattice dynamics coupled to the intra dimer degree of freedom in the organic charge transfer salts κ-(BEDT-TTF) <sub>2</sub> X with X=Cu[N(CN) <sub>2</sub> ]Cl and Cu <sub>2</sub> CN <sub>3</sub> | 21 |
| <a href="#">C-4</a>                                         | 17:25 | 17:45    | Contributed | Satoshi Iguchi    | IMR                             | Infrared Magneto-optical Kerr Effect in Anisotropic Materials                                                                                                                                       | 22 |
| <a href="#">C-5</a>                                         | 17:45 | 18:05    | Contributed | Shojiro Kimura    | IMR                             | Magnetic excitation in the S = 1/2 Ising-like antiferromagnetic chain in high magnetic fields                                                                                                       | 23 |
|                                                             | 18:05 | 18:20    | Break       |                   |                                 |                                                                                                                                                                                                     |    |
|                                                             | 18:20 | 19:40    | Mixer       |                   |                                 |                                                                                                                                                                                                     |    |



## Day 2: Nov. 21

| Number                                                                          | Time  |       | Category                                                       | Name                 | Affiliation                   | Title                                                                                                                                                                            | Page |
|---------------------------------------------------------------------------------|-------|-------|----------------------------------------------------------------|----------------------|-------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|
| Session D Material Design and Informatics (Chair: Momoji Kubo, IMR)             |       |       |                                                                |                      |                               |                                                                                                                                                                                  |      |
| <a href="#">D-1</a>                                                             | 9:30  | 10:00 | Invited                                                        | Talat S. Rahman      | University of Central Florida | Excited state charge dynamics and optical response of 2D materials: the role of phonons                                                                                          | 25   |
| <a href="#">D-2</a>                                                             | 10:00 | 10:20 | Contributed                                                    | Yu Kumagai           | IMR                           | Alkali mono-pnictides: a new class of photovoltaic materials by element mutation                                                                                                 | 26   |
| <a href="#">D-3</a>                                                             | 10:20 | 10:40 | Contributed                                                    | Goro Miyamoto        | IMR                           | Nano-sized Precipitates for Strengthening of Steels                                                                                                                              | 27   |
| <a href="#">D-4</a>                                                             | 10:40 | 11:00 | Contributed                                                    | Yusuke Ootani        | IMR                           | Frictional Property of Concentrated Polymer Brush Elucidated by Molecular Dynamics Simulation                                                                                    | 28   |
| <a href="#">D-5</a>                                                             | 11:00 | 11:20 | Contributed                                                    | Akarsh Verma         | Osaka University              | Stepped (coherent-incoherent) grain boundary in miscible random alloys: Elucidating the mechanical response effect                                                               | 29   |
| <a href="#">D-6</a>                                                             | 11:20 | 11:30 | Short                                                          | Shota Ono            | IMR                           | Stable configuration of 2D Cu <sub>16-x</sub> Au <sub>x</sub> : First-principles calculations, Bayesian optimization, and Lennard-Jones model                                    | 30   |
|                                                                                 | 11:30 | 12:45 | Lunch                                                          |                      |                               |                                                                                                                                                                                  |      |
|                                                                                 | 12:45 | 13:00 | Photo Session @Front Lobby of IMR Building 1 (A06)             |                      |                               |                                                                                                                                                                                  |      |
| Session E Spintronics and Topological Phenomena (Chair: Atsushi Tsukazaki, IMR) |       |       |                                                                |                      |                               |                                                                                                                                                                                  |      |
| <a href="#">E-1</a>                                                             | 13:00 | 13:30 | Invited                                                        | Takahiro Moriyama    | Nagoya University             | Electrical detection of antiferromagnetic dynamics: toward THz spectroscopy for nano-scale antiferromagnets                                                                      | 32   |
| <a href="#">E-2</a>                                                             | 13:30 | 14:00 | Invited                                                        | Ryusuke Matsunaga    | The University of Tokyo       | Dynamical aspect of Hall conductivity in topological antiferromagnet Mn <sub>3</sub> Sn studied by terahertz spectroscopy                                                        | 33   |
| <a href="#">E-3</a>                                                             | 14:00 | 14:20 | Contributed                                                    | Takeshi Seki         | IMR                           | Magneto-thermoelectric conversion in metallic superlattices                                                                                                                      | 34   |
| <a href="#">E-4</a>                                                             | 14:20 | 14:40 | Contributed                                                    | Motoi Kimata         | IMR                           | Enhancement of anomalous Hall effect at the vicinity of field-reentrant superconducting phase in the spin-triplet superconductor UTe <sub>2</sub>                                | 35   |
| <a href="#">E-5</a>                                                             | 14:40 | 15:00 | Contributed                                                    | Hidetoshi Masuda     | IMR                           | Helimagnet-based Spintronics: Control and Detection of Magnetic Chirality                                                                                                        | 36   |
| <a href="#">E-6</a>                                                             | 15:00 | 15:20 | Contributed                                                    | Michael Zhitomirsky  | CEA* & ICC-IMR*               | Magnetic frustration in octahedral networks: from antiperovskites to fcc antiferromagnets                                                                                        | 37   |
| <a href="#">E-7</a>                                                             | 15:20 | 15:30 | Short                                                          | Yusuke Kousaka       | Osaka Metropolitan University | Chiral Helimagnetism and Chiral Soliton Lattice in a Transition-Metal Dichalcogenide MnTa <sub>3</sub> S <sub>6</sub>                                                            | 38   |
|                                                                                 | 15:30 | 15:50 | Break                                                          |                      |                               |                                                                                                                                                                                  |      |
| Session F Functional Materials (Chair: Rie Y. Umetsu, IMR)                      |       |       |                                                                |                      |                               |                                                                                                                                                                                  |      |
| <a href="#">F-1</a>                                                             | 15:50 | 16:20 | Invited                                                        | Ratnamala Chatterjee | IIT Delhi*                    | Evidence for 2k <sub>F</sub> and 4k <sub>F</sub> incommensurate charge density wave in Ta <sub>2</sub> NiSe <sub>7</sub> single crystal through electrical and thermal transport | 40   |
| <a href="#">F-2</a>                                                             | 16:20 | 16:50 | Invited                                                        | Hidenori Fujiwara    | Osaka University              | Resonant inelastic soft x-ray scattering on spintronic materials                                                                                                                 | 41   |
| <a href="#">F-3</a>                                                             | 16:50 | 17:20 | Invited                                                        | Carmine Senatore     | University of Geneva          | Current Trends and Future Prospects for the High-Field Applications of Nb <sub>3</sub> Sn and REBCO Superconductors                                                              | 42   |
| <a href="#">F-4</a>                                                             | 17:20 | 17:40 | Contributed                                                    | Tatsunori Okada      | IMR                           | Critical current characterization using high-field cryogen-free superconducting magnets at HFLSM                                                                                 | 43   |
| <a href="#">F-5</a>                                                             | 17:40 | 18:00 | Contributed                                                    | Hanae Kijima-Aoki    | Tohoku University             | Multifunctionality via spin-dependent tunneling in magneto-dielectric nanocomposite thin films                                                                                   | 44   |
| <a href="#">F-6</a>                                                             | 18:00 | 18:20 | Contributed                                                    | Kazuki Ohishi        | CROSS*                        | Ion Dynamics in Na-Ion Battery Materials Studied by SANS and $\mu$ SR                                                                                                            | 45   |
|                                                                                 | 18:20 | 19:40 | Poster Session @Front Lobby and Lounge of IMR Building 2 (A07) |                      |                               |                                                                                                                                                                                  |      |

## Day 3: Nov. 22

| Number                                                                            | Time  | Category | Name        | Affiliation            | Title                                        | Page                                                                                                                             |    |
|-----------------------------------------------------------------------------------|-------|----------|-------------|------------------------|----------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|----|
| Session G Nuclear and Irradiation (Chair: Yasuyoshi Nagai, IMR)                   |       |          |             |                        |                                              |                                                                                                                                  |    |
| <a href="#">G-1</a>                                                               | 9:30  | 10:00    | Invited     | Somei Ohnuki           | University of Science and Technology Beijing | Phase separation and damage structure in Fe-Cr alloys under neutron-irradiation                                                  | 47 |
| <a href="#">G-2</a>                                                               | 10:00 | 10:30    | Invited     | Takuji Oda             | Seoul National University                    | Atomistic simulation of hydrogen isotope diffusion in metals using machine-learning interatomic potentials                       | 48 |
| <a href="#">G-3</a>                                                               | 10:30 | 10:50    | Contributed | Sosuke Kondo           | IMR                                          | Process Informatics for CVD Coating on SiC/SiC for Nuclear Applications                                                          | 49 |
| <a href="#">G-4</a>                                                               | 10:50 | 11:10    | Contributed | Koji Inoue             | IMR                                          | Evolution of Ni-Mn-Si clusters in a low copper reactor pressure vessel steel analyzed by atom probe tomography                   | 50 |
| <a href="#">G-5</a>                                                               | 11:10 | 11:30    | Contributed | Steven Van Dyck        | SCK-CEN*                                     | Study of neutron irradiation effects in materials using the BR2 material test reactor                                            | 51 |
|                                                                                   | 11:30 | 11:40    | Break       |                        |                                              |                                                                                                                                  |    |
| Session H Advanced Metallurgy-3D Printing and Nanomaterials (Chair: Sosuke Kondo) |       |          |             |                        |                                              |                                                                                                                                  |    |
| <a href="#">H-1</a>                                                               | 11:40 | 12:10    | Invited     | Christopher Hutchinson | Monash University                            | Nucleation in solid state phase transformations requiring a change in chemistry                                                  | 53 |
| <a href="#">H-2</a>                                                               | 12:10 | 12:40    | Invited     | Mari Onodera           | Panasonic Industry Co., Ltd.                 | Development of Multi-Layered Cosmetic Sheet Applied by Printed Electronics Technology                                            | 54 |
|                                                                                   | 12:40 | 13:40    | Lunch       |                        |                                              |                                                                                                                                  |    |
| <a href="#">H-3</a>                                                               | 13:40 | 14:10    | Invited     | Naoki Tarutani         | Hiroshima University                         | Thermal conversion of metal hydroxide salt nanoparticles towards nanoparticulate and porous structured alloy materials           | 55 |
| <a href="#">H-4</a>                                                               | 14:10 | 14:30    | Contributed | Kenta Aoyagi           | IMR                                          | In-process monitoring for electron beam powder bed fusion by using electron beam imaging technology                              | 56 |
| <a href="#">H-5</a>                                                               | 14:30 | 14:40    | Short       | Zhenxing Zhou          | Tohoku University                            | Fabrication of refractory alloy by freeze-dry pulsated orifice ejection method and laser powder bed fusion                       | 57 |
|                                                                                   | 14:40 | 15:00    | Break       |                        |                                              |                                                                                                                                  |    |
| Session I Hydrogen Materials (Chair: Eiji Akiyama, IMR)                           |       |          |             |                        |                                              |                                                                                                                                  |    |
| <a href="#">I-1</a>                                                               | 15:00 | 15:30    | Invited     | Kohta Asano            | AIST*                                        | Nano-structural configuration of destabilized Mg hydride for hydrogen storage materials                                          | 59 |
| <a href="#">I-2</a>                                                               | 15:30 | 15:50    | Contributed | Shigeyuki Takagi       | IMR                                          | Creation and functionalization of hydride complexes with high hydrogen coordination                                              | 60 |
| <a href="#">I-3</a>                                                               | 15:50 | 16:10    | Contributed | Hiroshi Kakinuma       | IMR                                          | Filming microstructure-dependent hydrogen diffusion in polycrystalline metals using a hydrogen video imaging system              | 61 |
| <a href="#">I-4</a>                                                               | 16:10 | 16:20    | Short       | Ruirui Song            | IMR                                          | Ultrafine Nanoporous Intermetallic Catalysts by High-Temperature Liquid Metal Dealloying for Electrochemical Hydrogen Production | 62 |
|                                                                                   | 16:20 | 16:50    | Closing     |                        |                                              |                                                                                                                                  |    |

## Poster Session

| Number               | Name                 | Affiliation             | Title                                                                                                                                                                                                              | Page |
|----------------------|----------------------|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|
| <a href="#">PS1</a>  | Xiaoyang Zheng       | NIMS*                   | Deep Learning in Mechanical Metamaterials                                                                                                                                                                          | 64   |
| <a href="#">PS2</a>  | Shigeru Suzuki       | Tohoku University       | Vibration Energy Harvesting using Electromagnetic Induction Assisted by Inverse Magnetostriction of Iron-based Alloys                                                                                              | 65   |
| <a href="#">PS3</a>  | Kohei Fujiwara       | IMR                     | Reducing the conducting channel thickness of ferromagnetic $\text{Co}_3\text{Sn}_2\text{S}_2$ films by bias-induced dealloying                                                                                     | 66   |
| <a href="#">PS4</a>  | Rayko Simura         | Tohoku University       | In-house single crystal X-ray diffraction measurement system with anomalous X-ray scattering for site-selective structure analysis                                                                                 | 67   |
| <a href="#">PS5</a>  | Dayal Chandra Roy    | Iwate University        | Investigation and characterization of rare-earth free double-perovskite oxides $\text{Ba}_2\text{Bi}^{3+}(\text{Bi}_{1-2x}^{5+}\text{Sb}_{2x}^{5+})\text{O}_6$ : A comparative study of photocatalytic performance | 68   |
| <a href="#">PS6</a>  | Takeshi Hagiwara     | Kanagawa University     | Syntheses and some properties of $\text{AlLB}_{14}$ ( $L = \text{Li, Na}$ ) crystals by Al self-flux                                                                                                               | 69   |
| <a href="#">PS7</a>  | Teruhito Nakashita   | The University of Tokyo | Search for fundamental symmetry by trapping francium atoms                                                                                                                                                         | 70   |
| <a href="#">PS8</a>  | Kenji Ishii          | QST*                    | Post-growth annealing effects on charge and spin excitations in $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ studied by resonant inelastic x-ray scattering                                                            | 71   |
| <a href="#">PS9</a>  | Vu Thi Ngoc Huyen    | IMR                     | Piezomagnetic effect in $\text{Mn}_3\text{AN}$ and $\text{Mn}_3\text{X}$ from symmetry analysis and first-principles calculations                                                                                  | 72   |
| <a href="#">PS10</a> | Kyosuke Sakurai      | IMR                     | Metal-insulator transition behavior of $\text{RECoO}_3$ for high field superconducting magnets                                                                                                                     | 73   |
| <a href="#">PS11</a> | Shogo Yoshida        | Kogakuin University     | Growth of $\text{Cu}_3\text{N}$ Films by Mist CVD with Ethylenediamine                                                                                                                                             | 74   |
| <a href="#">PS12</a> | Kaoru Kouzu          | Kokushikan University   | Syntheses and some properties of $R(\text{Al,W})\text{B}_4$ ( $R = \text{rear earth}$ ) compounds                                                                                                                  | 75   |
| <a href="#">PS13</a> | Kushwaha Varun Kumar | IMR                     | Selective magnetization switching conditions for hard magnetic $\text{FePt}$ with spin-wave dynamics                                                                                                               | 76   |
| <a href="#">PS14</a> | Keita Ito            | IMR                     | Correlation between magnetostriction and magnetic damping in $\text{Fe}_{4-x}\text{Mn}_x\text{N}$ and $\text{Fe}_{4-y}\text{Co}_y\text{N}$ films                                                                   | 77   |
| <a href="#">PS15</a> | Yoshihiko Umemoto    | IMR                     | Local Structure Analysis of Iron-Manganese-Based Elinvar Alloys via Neutron Total Scattering                                                                                                                       | 78   |
| <a href="#">PS16</a> | Ta-Te Chen           | Nagoya University       | Estimation of plastic properties of alloys using instrumented indentation test                                                                                                                                     | 79   |

AIST: National Institute of Advanced Industrial Science and Technology  
 CEA: Commissariat à l'énergie atomique et aux énergies alternatives  
 CROSS: Comprehensive Research Organization for Science and Society  
 ICC-IMR: International Collaboration Center, Institute for Materials Research, Tohoku University  
 IIT Delhi: Indian Institute of Technology Delhi  
 NIMS: National Institute for Materials Science  
 QST: National Institutes for Quantum Science and Technology  
 SCK-CEN: Belgian Nuclear Research Centre

Activity Report

# Young Researcher Fellowships



### Young Researcher Fellowships

| No.   | Title         | Applicant                 | Affiliation                              | Host Professor          | Proposed Research                                                                                      | Term                 |
|-------|---------------|---------------------------|------------------------------------------|-------------------------|--------------------------------------------------------------------------------------------------------|----------------------|
| 23FS1 | Ph.D. Student | Mochammad Yan Pandu Akbar | Institut Teknologi Bandung, Indonesia    | Prof. Fujita            | Investigation of Crystal and Magnetic Structure of $\beta$ -NaFeO <sub>2</sub> Single Crystal          | 2023.10.9-2023.12.9  |
| 23FS2 | Ph.D. Student | Gabriela Kamila Handzlik  | Jagiellonian University, Poland          | Prof. Miyasaka          | Magnetic Circular Dichroism Measurements for Complexes Based on Lanthanide Ions and Helicenes          | 2023.10.27-2023.12.2 |
| 23FS3 | Ph.D. Student | Oliver Jack Dowinton      | University of Manchester, UK             | Assoc. Prof. Belosludov | First-Principles Modelling of Spin Transport in Low-Dimensional Cross-Correlated Materials             | 2023.7.30-2023.9.2   |
| 23FS4 | Ph.D. Student | Basit Ali                 | Technical University of Denmark, Denmark | Prof. Furuhashi         | (HR)TEM Characterization of Martensite Formation in Nitrogen-Stabilized Precipitation Hardenable Steel | 2023.8.23-2023.11.5  |



## Investigation of magnetic structures of $\beta$ -NaFeO<sub>2</sub> Single Crystal

The magnetization measurement on  $\beta$ -NaFeO<sub>2</sub> single crystal shows a transition at 120 K. Single crystal neutron diffraction reveals incommensurate peaks, suggesting an incommensurate spin structure. To investigate this structure, we attempted to grow more crystals for neutron experiment. However, further investigations into the low-temperature magnetic structures is challenging due to unstable growth parameters.

NaFeO<sub>2</sub> is crystallized in three different structures namely  $\alpha$ ,  $\beta$ , and  $\gamma$ -phase.  $\alpha$ -NaFeO<sub>2</sub> is an antiferromagnet that has a rock-salt type crystal structure with  $R\bar{3}m$  space group similar to the multiferroic delafosite CuFeO<sub>2</sub>. Systematic analyses by means of magnetization measurement and neutron diffraction revealed rich magneto-electric phase diagrams [1,2].  $\beta$ -NaFeO<sub>2</sub> is also an antiferromagnet with  $T_N \sim 720$  K [3]. However, compared to the  $\alpha$ -phase, the magnetic orderings in  $\beta$ -NaFeO<sub>2</sub> are still unexplored.

In our previous work, we obtained a single crystal of  $\beta$ -NaFeO<sub>2</sub> using the floating zone method. Careful characterizations on this crystal revealed a single-phase compound with an orthorhombic structure belonging to  $Pna2_1$  space group.

Magnetization measurement on this crystal from 400 K to 3 K revealed several transitions, namely two kinks at around 120 K and 20 K which were observed along  $a$  and  $b$ -axes. The kink at 120 K is absent in  $c$ -axis. These anomalies hint at a magnetic transition that to our knowledge has not been reported yet.

In order to investigate these anomalies, we performed single crystal diffraction using AKANE facility in JRR-3 in collaboration with the group of Prof. M. Fujita. At room temperature, there are three magnetic reflections labeled as (100), (101), and (020). By scanning the momentum diagonally around (101) peak we revealed three incommensurate peaks as shown in Fig. 2 (a). These peaks were fitted using Gaussian function. We find that the position of the peak  $q_2$  and  $q_3$  remain unchanged with temperature. Interestingly, the position of  $q_1$  changes at around 140 K. This temperature is close to the observed high-temperature kink in magnetization data as shown in Fig. 2(b). Such a feature indicates an incommensurate spin structure.

To get more insight into this magnetic structure, we need to get information about the low-temperature magnetic structures of this compound. To do this we attempted to grow more single crystals in Institute Materials Research, Tohoku University, Sendai. The growth was performed using floating zone

technique following the growth parameters we used before. We obtained several crystal boules with typical lengths of 20 mm and diameters of 5 mm. The XRD indicates a single-phase material. However, the Laue image taken for several crystal boules from different batches show an unclear reflection pattern. This indicates the quality of the crystal is still not so good compared to the one we used for neutron diffraction measurement. Possibly, this is due to the unstable growth parameters. These results make further investigation on the magnetic structure still inaccessible and thus further attempts at crystal growth are necessary in the future.

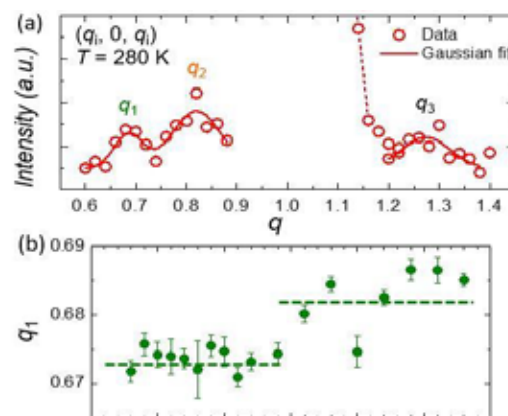


Fig. 1 (a) neutron diffraction pattern taken from AKANE in JRR-3 and (b) temperature-dependent  $q_1$ .

Keywords: crystal growth, neutron diffraction, magnetic structure

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## Activity report for the research proposal "Magnetic circular dichroism measurements for complexes based on lanthanide ions and helicenenes"

A research visit to the Miyasaka Laboratory within the ICC-IMR Fellowship for Young Scientists gave the opportunity to perform magnetic circular dichroism (MCD) measurements for complexes based on lanthanide ions and helicenenes prepared in the Pinkowicz Group. MCD spectra were measured in the UV-Vis region in a series of magnetic fields and temperatures. Particularly interesting results were obtained for the erbium complex with azahelicene.

During a one-month research visit (2023.10.27-2023.12.02) to the Laboratory of Prof. Hitoshi Miyasaka, a series of lanthanide-based compounds were screened to find the best candidates for more detailed magnetic circular dichroism (MCD) measurements. The compounds for the study included a series of optically pure complexes with the smallest helicene -  $\{\Delta\text{-}[\text{Ln}(\text{phendo})_4]\}\{\Delta\text{-}[\text{As}(\text{cat})_3]_2(\text{NO}_3)\cdot 5\text{MeCN}\Delta\text{-Ln}$  (Ln = Gd, Tb, Dy, Ho, Er, Yb; phendo = 1,10-phenanthroline-N,N'-dioxide; cat = catecholate dianion) as well as the ( $\Lambda$ ,  $\Lambda$ ) forms (**LnAsphendo**) and optically pure complexes with a larger helicene ligand -  $[\text{Er}(\text{BHT})_3]_2((M/P)\text{-azahelicene})$  (BHT = butylated hydroxytoluene anion; azahelicene = benzo[4,5]imidazo[1,2-a]benzo[4,5]imidazo[2,1-k][1,10]phenanthroline) (**Er<sub>2</sub>azahel**).

Each sample was ground to fine powder and mixed with Apiezon® grease. The thin layer of such a mixture was placed between two BaF<sub>2</sub> windows. All operations for **Er<sub>2</sub>azahel** were carried out under an inert atmosphere, since erbium ions in this complex have an unsaturated coordination sphere and are prone to coordination of additional water or other solvent molecules. NCD (natural circular dichroism) and MCD spectra of BaF<sub>2</sub> windows with pure Apiezon® grease were also measured to exclude any signals from these components.

For one enantiomer of each complex (7 compounds in total), NCD (without magnetic field) and MCD (at  $\pm 1.5$  T) were measured at 5 K. Complete MCD study was performed only for the most promising compounds (both enantiomers). The full MCD study included measurements of the field dependence of the spectrum at 5 K (from -1.5 T to +1.5 T), a more precise study of the field dependence of the MCD signals at certain wavelengths (in maxima) and the temperature dependence of the MCD spectra (5-300 K).

Among the **LnAsphendo** complexes, Er- and Dy-based compounds show MCD signals (at 519.5 nm and 314 nm, respectively). Unfortunately, the signals for both compounds are quite weak and visible only at very low temperature. On the other hand, the MCD spectrum for **Er<sub>2</sub>azahel** shows really strong signals (maxima at: 376, 380, 517, 522 and 525 nm) that are visible up to room temperature. Fig. 1 shows the MCD spectra of the M enantiomer of **Er<sub>2</sub>azahel**, extracted from the measured combination of NCD and MCD. The temperature dependence of the MCD signal is compared with the absorption spectra of unpolarized light for **Er<sub>2</sub>azahel** and ErCl<sub>3</sub>. Based on this comparison, one can say which erbium transitions are active in MCD ( $^4\text{I}_{15/2} \rightarrow ^4\text{G}_{11/2}$  and  $^4\text{I}_{15/2} \rightarrow ^2\text{H}_{11/2}$ ).

The results of these measurements will complete the full magneto-chiral characteristic of the obtained compounds: NCD, MCD and magneto-chiral dichroism (MChD). We already have preliminary results of MChD measurements from the collaboration with Dr. Matteo Atzori (LNCMI, CNRS, Grenoble, France).

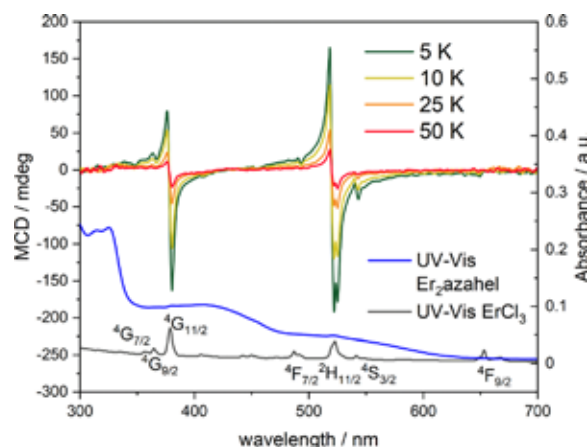


Fig. 1 Magnetic circular dichroism spectra of  $[\text{Er}(\text{BHT})_3]_2((M)\text{-}(-)\text{-azahelicene})$  compared with UV-Vis spectra of **Er<sub>2</sub>azahel** and ErCl<sub>3</sub> salt.

Keywords: optical properties, magnetic properties, lanthanide  
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## Magnetically Controllable Two-Dimensional Spin Transport in a Three-Dimensional Crystal

Intrinsic crystal anisotropy in a “fractional” perovskite,  $\text{Eu}_x\text{TaO}_3$  ( $x = 1/3 \sim 1/2$ ), is predicted theoretically to lead to stacked layers of quasi-2D electron gases (2DEG), despite being a three-dimensional bulk system. A non-monotonic thermopower is proposed as a route to experimentally demonstrate the quasi-2D behavior.

The exploration of two-dimensional (2D) states has come to such prominence in condensed matter and materials research because their properties make them desirable, or even essential, for state of the art device applications. From ab-initio calculations, analytic toy models, and group theoretic arguments we were able to show  $\text{Eu}_x\text{TaO}_3$ , a fractional rare-earth transition metal perovskite with  $x = 1/3 \sim 1/2$ , naturally exhibits quasi-2DEGs stacked along its crystalline c-axis, as shown in Fig 1, despite it being a bulk 3D material[1].

An interplay between the underlying tetragonal crystal field (TCF) with the spin-orbit coupling (SOC) of the Ta sites and their exchange coupling with local Eu magnetic moments, leads to quasi-2D conduction bands of a single orbital character, spin-polarized along the magnetic axis. These bands have additional in-plane spin textures that have a topological monopole(anti-monopole) form, which arises from a coupling between two component Rashba fields[2], Fig1, and the strong SOC of the carriers.

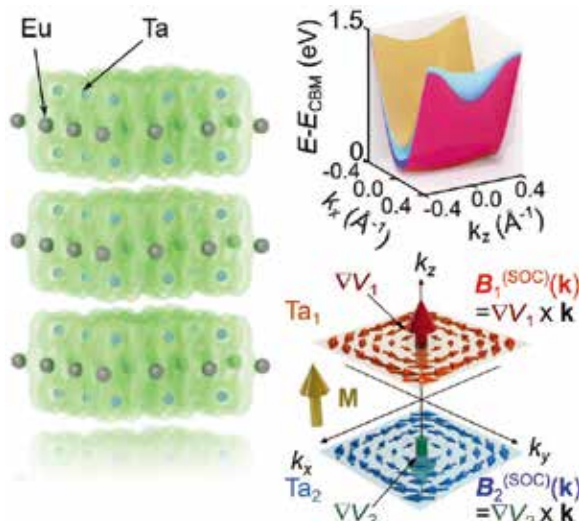


Figure 1 The charge density of quasi-2DEG phase, the quasi 2D conduction band dispersion, and component Rashba spin textures.

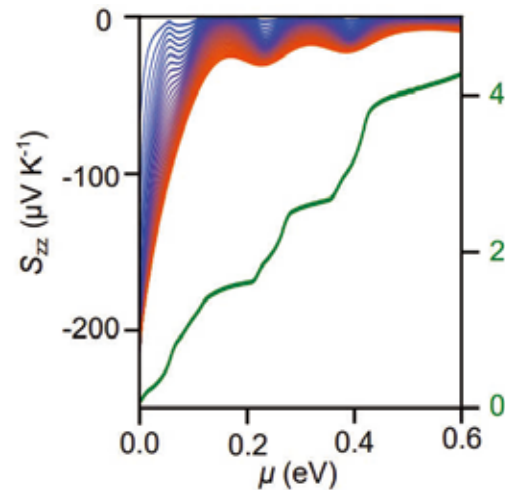


Figure 1 The Oscillating Seebeck coefficient, the arises from the quasi-2D DOS of the conduction bands as shown.

As the magnetic ordering of the charge carriers arises indirectly from an exchange interaction with Eu, these spin textures can be externally manipulated, for example, by the magnetic field orientation, without any change in their Fermiology. This makes  $\text{Eu}_x\text{TaO}_3$  a promising platform for a broad range of spintronic devices.

We went on to examine possible quantum states arising from this quasi-2D behaviour, and proposed methods to experimentally investigate them. In particular, an oscillatory Seebeck effect that deviates from typical metallic behaviour due to plateaus in the density of states (DOS)[3] as shown in Fig 2. We propose that this may be utilizable as a thermoelectric source with robust spin and orbital characters.

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Keywords: Spintronic, Thermoelectric, Magnetism

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## TEM characterization of martensite formation in nitrogen-stabilized precipitation hardenable steel

Martensite formation at sub-zero Celsius temperatures in nitrogen-added 17-4 PH stainless steel was studied. Two transformation conditions, namely athermal and isothermal, were tested. Samples transformed athermally showed plate-type martensite, whereas samples transformed isothermally exhibited typical lath-type martensite. The results reveal a connection between microstructure and the kinetics of martensite formation.

Precipitation-hardenable 17-4 PH martensitic stainless steel, belonging to a class of structural metastable stainless steels, is favored in the additive manufacturing (AM) industry [1]. Literature indicates that samples produced from nitrogen-atomized 17-4 PH powders exhibit a high amount of retained austenite in their microstructure [2], which influences strength by regulating the kinetics of martensite transformation. Consequently, there is a growing interest in understanding the effect of nitrogen on austenite stability and martensite formation in this steel. Research has demonstrated that martensite can form isothermally at sub-zero Celsius temperatures, challenging the conventional belief that martensite solely undergoes athermal transformation. Furthermore, suggestions have been made regarding the distinct morphologies of athermal and isothermal martensite [3].

The current study investigated this hypothesis by altering the martensite start temperature,  $M_s$ , of commercial 17-4 PH through control of interstitial nitrogen content via a high-temperature solution nitriding (HTSN) process, bringing  $M_s$  into the sub-zero Celsius range. For this investigation, the nitrogen content was fixed at 0.12 wt%. Two samples were prepared: one sample was quenched in liquid nitrogen (athermal), while the second sample underwent isothermal transformation at 210 K for 2 days. In-situ vibrating sample magnetometry (VSM) was employed to monitor the isothermal martensite formation, revealing a martensite fraction of approximately 5 vol%. The microstructure of the transformed samples was examined using electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM). TEM specimens were prepared through focused ion beam (FIB) lift-out, highlighting areas in the EBSD maps. Additionally, TEM analysis included bright and dark-field imaging, along with diffraction. Results are depicted in Fig. 1.

A clear difference in microstructure between the athermal and isothermal

samples was observed, with the athermal sample exhibiting a plate-type morphology, as evident from the dark-field (DF) images of TEM, whereas the sample transformed isothermally displayed a typical lath-type morphology with thin layers of austenite sandwiched between martensite laths (cf. TEM results). These results indicate that martensite formation at sub-zero Celsius temperatures is thermally activated. The current investigation highlights a clear connection between the kinetics of martensite formation and the resulting martensite morphology, suggesting that isothermal or thermally activated martensite formation in steels is more of a rule than an exception.

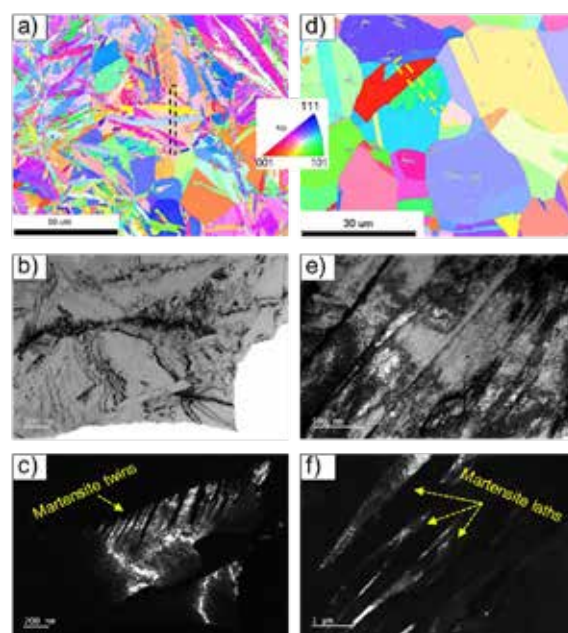


Fig 1: a-c) EBSD and TEM results of martensite formed in sample athermally transformed by quenching in liquid nitrogen, and d-f) for sample transformed isothermally at 210 K for 2 days.

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## Activity Report

# Oversea Visit for IMR Young Researchers





### Oversea Visit for IMR Young Researchers

| No.   | Title         | Applicant | Name of Institution or Conference visited                               | Supervisor   | Proposed Research                                                                                                                 | Term               |
|-------|---------------|-----------|-------------------------------------------------------------------------|--------------|-----------------------------------------------------------------------------------------------------------------------------------|--------------------|
| 23IS1 | Ph.D. Student | Xie Peiao | The 24th European Conference on Fracture (ECF24), Villigen, Switzerland | Prof. Fujita | Resonant Inelastic X-Ray Scattering Study on Charge Density Order in T*-Type High-Transition-Temperature Cuprate Superconductors. | 2023.8.26-2023.9.7 |

Temperature dependence resonant inelastic X-ray scattering study on charge density order in T\*-type copper-based superconductors.

In this report, we studied the temperature dependence charge order feature for the 214-type T\* phase SLSCO through the RIXS technique. We observed a markedly different evolution of the charge order wavevector in SLSCO compared to that of traditional 214-type cuprates. Additionally, we noted a potential distinction between the combined CDW+CDF mixture and an isolated CDF signal.

In cuprate research, the different phases within the pseudogap region have consistently drawn significant interest from scientists. The charge order phenomenon is a hot topic in current discussions [1]. Recently, the resonant inelastic X-ray scattering (RIXS) studies revealed that very short-range charge order called charge density fluctuation (CDF) is almost ubiquitously observed at high temperatures for all cuprates [2][3]. In this report, we studied the temperature dependence feature of the charge order of the long-time left-visited 214-type T\* phase cuprate  $\text{SmLa}_{0.75}\text{Sr}_{0.25}\text{CuO}_4$  (SLSCO) for the first time. Our prior ARPES studies estimate an effective hole concentration of  $\sim 10\%$  in this sample [4]. The experiment is performed at ADRESS-RIXS, Swiss Light Source (SLS), Paul Scherrer Institute (PSI), Switzerland.

Fig.1 shows the temperature dependence integral intensity of the quasi-elastic peaks along the  $(h, 0)$  direction plotted as the dotted data. The colorful solid line represents the fitting results obtained using the Lorentzian profile. The peak position centered at  $h \sim 0.29$ , except 250 and 290 K, caused by the strong background that affected the fitting. Figure 2 displays the peak heights and widths (full width at half maximum). It is evident that the peak height decreases steadily, while a clear "kink" in the

peak width emerges near 100 K.

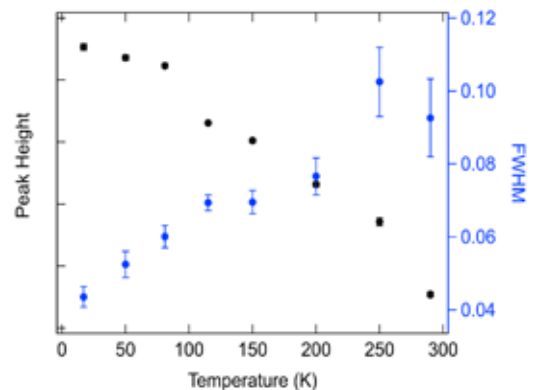


Fig. 2 Peak height and FWHM against temperatures.

The results indicate that the charge order wavevector's position in SLSCO deviates from that of conventional 214-type cuprates, which are closer to the non-214-type families [5]. A potential reason could be the significantly weaker magnetism in T\* phase cuprates, which disrupts the coupling between spin and charge order, leading to a conventional charge density wave (CDW) instead of stripe order. We conclude that two similar peaks also appeared in our samples: the broad CDF peak and the narrow CDW peak. This assumption could be reflected in the distinct evolution of the peak width at  $\sim 100$  K, which could be attributed to the separation of the mixture CDW+CDF and single CDF state. However, cause of the limited Instrument resolution in ADRESS-RIXS ( $\sim 122$  meV), we couldn't detect the additional peak in the current results. An improved high-resolution RIXS experiment is needed.

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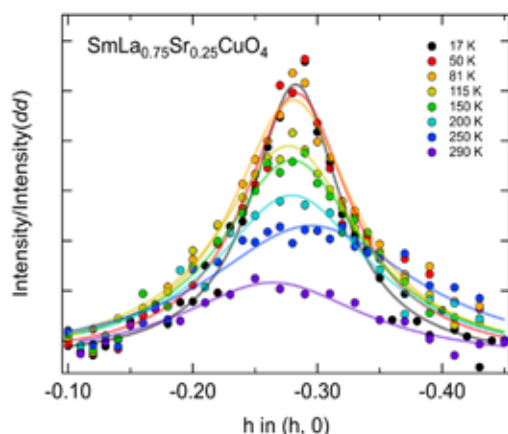


Fig. 1 Integral intensity of quasi-elastic peaks.

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## ICC-IMR FY2023 Activity Report

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