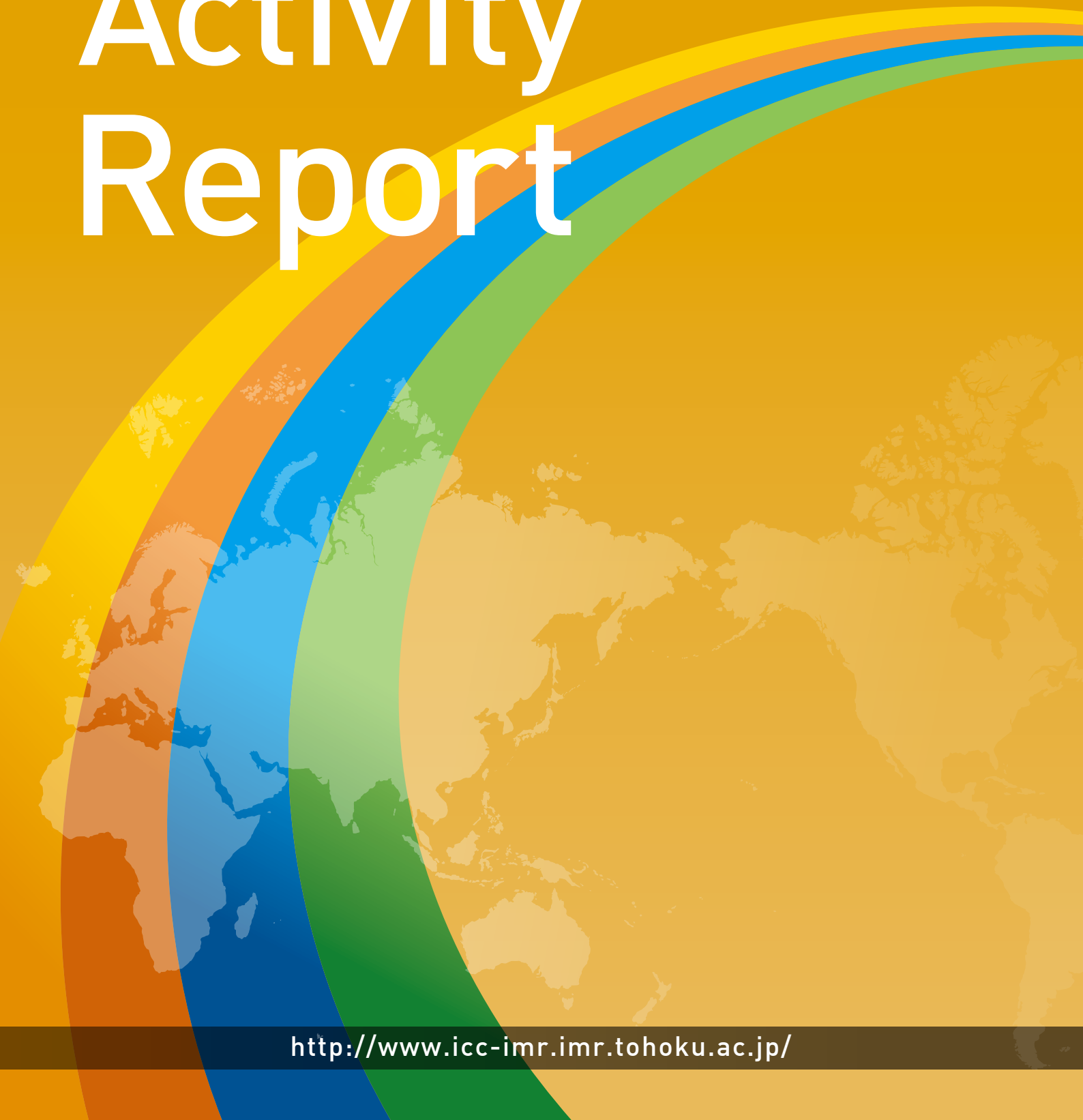
International Collaboration Center
Institute for Materials Research
Tohoku University
ICC-IMR

ICC-IMR FY2022 Activity Report



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ICC-IMR FY2022

Activity Report

International Collaboration Center

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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 77 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

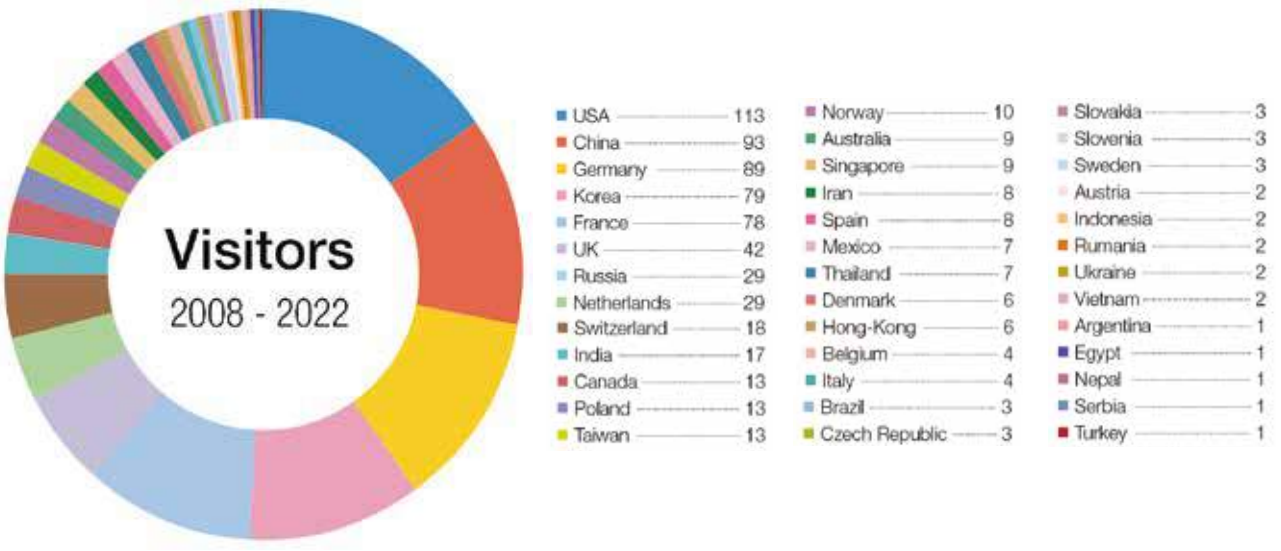
3) International Workshops

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
21G02	Visiting Associate Professor	Arnaud Joel Badel	CNRS, France	Prof. Awaji	High Temperature Superconductors for Very High Field Magnets Beyond 30T	2022.4.9-4.21 2022.7.5-7.25
22G01	Visiting Professor	Farhad Rezai-Aria	Institut Mines-Télécom, É cole Nationale Supérieure des Mines d'Albi-Carmaux, Institut Clément Ader Site - Albi, France	Prof. Chiba	TA2M5: Thermomechanical Assessments of Additively Manufactured Metallic Materials & Multi-Materials	2022.6.6-8.5
22G02	Visiting Professor	Hidekazu Kurebayashi	University College London, U.K.	Assoc. Prof. Seki	Fabricating Marmin Wagner Magnets by State-of-the-Art Thin-Film Growth Techniques	2022.7.1-8.31
22G03	Visiting Professor	Sanjit Konar	Indian Institute of Science Education and Research (IISER) Bhopal, India	Prof. Miyasaka	Design of Redox-Active Porous Molecular Materials for Guest Induced Controlling of Electron Conduction and Magnetic Properties	2022.5.9-6.8
22G04	Visiting Associate Professor	Rasmus Toft-Petersen	Technical University of Denmark	Prof. Nojiri	High-Field Magnetic Phase Transitions in Magnetoelectric Systems	2022.4.1-2022.12.1
22G05	Visiting Professor	Matthias Militzer	The University of British Columbia, Canada	Prof. Furuhara	Modelling of Alloying Element Interaction with Migrating Interfaces in Metals and Alloys	2022.7.11-9.9
22G06	Visiting Professor	Thierry Duffar	Grenoble Institute of Technology, France	Prof. Fujiwara	Growth Kinetics at Crystal/Melt Interface	2022.10.1-11.30
22G07	Visiting Associate Professor	Wojciech Gieszczyk	Institute of Nuclear Physics Polish Academy of Sciences, Poland	Prof. Yoshikawa	Dosimetry of Ionizing Radiation Using Stimulated Luminescence Phenomena	2023.1.16-4.14

Development of mechanically and electrically reliable isolated REBCO HTS coils with high current densities

REBCO Coated Conductors inserts are now widely considered as the solution for future very high field magnets, 30 T and beyond. Yet, the number of full-size HTS inserts tested worldwide is limited, and there is a lack of data regarding their reliability. In this work the mechanical and electrical behavior of a quasi-full scale REBCO insert made of 20 stacked pancakes was modelled, and results were compared with experimental data.

A robust REBCO insert coil concept was proposed recently at HFLSM [1], in the framework of the 30 T upgrade project. Its key features can be summarized as:

- Pancake-based solenoids with epoxy impregnation, using a non-stick material in between turns to ensure conduction-cooling efficiency and improve the winding stiffness.
- Fully isolated turns to limit the transient losses and to achieve fast dynamics. In this way, the insert can be discharged in a few seconds, as fast as the outsert, limiting energy transfer from one to the other during an outsert quench [2].
- Conductor formed of two REBCO tapes co-wound so that current can be shared [3] to reduce the risk posed by local defects.
- Protection against thermal runaway by using early detection of dissipative behaviour thanks to sensitive voltage detection, triggering discharge in dump resistor [2].

That concept was developed over the years with small-scale validation coils of gradually increasing size and performance at HFLSM with contribution of Neel Institute (Grenoble) for thermal runaway detection and management. A much larger size implementation was successfully tested under 14 T background, demonstrating the practical feasibility of high performance yet reliable REBCO full-size insert coils. It consists of 20 pancakes from the 30 T upgrade project wound using 4 mm-wide Fujikura tape (inner bore 68 mm, outer bore 266 mm, total tape length 5.8 km, inductance 2.63 H). At the nominal current of 300 A, it generates more than 11 T.

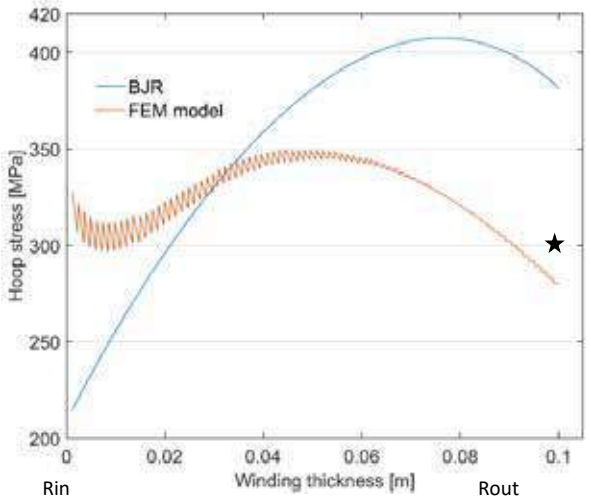

Fig. 1: Predicted Hoop Stress across the middle plane of the 20-stacked pancakes prototype at 300 A under 14 T background. Black star indicates estimated hoop stress based on strain measurement

The mechanical hoop stress was modelled using Finite Element Method, accounting for the specific structure of the edge-impregnated pancakes. The measured strain on outer diameter matches well with the value predicted by FEM, but not with the simpler "self-supporting turns" assumption (BJR formula), as shown Fig. 1. Following the FEM model, it is estimated that the circumferential elongation reached 0.25 % at maximum (corresponding to 350 MPa hoop stress), without observed degradation of the pancakes winding and their connections. In this condition (300 A under 14 T background), the centre field exceeded 25 T, with 25.25 T measured by hall sensor.

From the viewpoint of thermal runaway protection, the idea of multichannel monitoring using independent pick up coils [4] was used. The use of 5 channels monitoring 4 pancakes each offer a good sensitivity as well as to enable localization of potential weak areas. The tests were carried out at 4.2 K in LHe, so that the theoretical temperature margin was very large. No dissipative behaviour was observed, proving the good health of the windings. Yet, the acquired signals support the idea that if a dissipative area had appeared, it could have been detected early enough to prevent degradation of the windings. Indeed, Fig. 2 present the superposition of the acquired signals on one of the channels in the last minutes of the current ramp, with the predicted voltage in case of local defect using a detailed thermal runaway model as in [2]. The change of trend in case of a dissipative behaviour can clearly be identified more than 60 s before thermal runway would occur, leaving enough time to discharge the magnet safely. In recent unpublished work, this dissipative voltage detection was tested at higher temperature repeatedly without damage, further demonstrating the reliability of the robust REBCO insert coil concept.

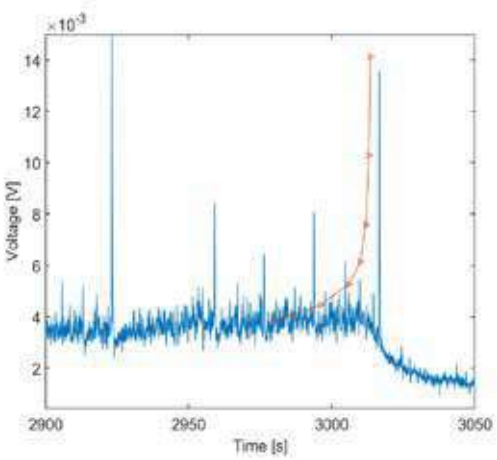

Fig. 2: Detail of the end of the current ramp reaching I=300 A under 14 T background field. In blue: experimental measurement of voltage signal using inductive compensation, across pancakes 1 to 4. In red: simulated quench behavior on a local hotspot gradually losing thermal balance for I=300 A [4].

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2 Keywords: High magnetic field, High Tc Superconductors
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Microstructural evolution at high temperature under two tensile strain rates of Ti6Al4V-Additively Layer Manufactured & 3D3C project preparation progress

High temperature tensile tests were first performed on TA6V4 fabricated by additive manufacturing of powder layers by laser fusion at Mines Albi-France.
The microstructural evolutions were then studied by EBSD, XY tomography and optical microscopy.at TLC-IMR.
The progress of the preparation of the Japan/France/Canada collaboration on ALM powder issues is reported.

I had the privilege to stay for 2 months (4 June-4 August 2022) in the laboratory of Professor Akihiko Chiba at IMR. The purpose of this stay was to consolidate exchanges on ALM with his laboratory, which is a major player in ALM. I was extremely impressed, although I expected it, by the breadth of ALM research topics covered by Professor Akihiko Chiba's team through the work of his colleagues and several of his superbly active students. I was able to visit very efficient facilities run by experienced and very competent staff. I was also very impressed when I visited with Professor Akihiko Chiba the JAMPT Corporation (Japan Additive Manufacturing Processing and Technology) centre and its president Ryota Kusaka. The resources that JAMPT has devoted to ALM in such a short period of time are a testament to the immense amount of work that is being done meticulously and efficiently.

I also had the opportunity and privilege to meet Professor Hiuoyuki Fukuyama and discuss his unique experiments and methods of measuring the physical properties of liquid phase martial metals by electromagnetic or electrostatic levitation. In situ neutron diffraction tensile tests (J-PARC) were initiated by Prof. Kenta Yamanaka on Ti6Al4V-ALM. During my stay, with the close collaboration of Dr. Sun Jiayu, we were able to work on the evolution of the microstructure (Fig. 1 & 2) and damage of this alloy during high temperature tensile tests (730°C and 840°C and strain rates of 10-2 and 10-4 (mm/mm)/s) carried out at Mines Albi in order to compare it to the behaviour of the ultrafine-grained Ti6Al4V alloy, which exhibits superplasticity at these temperatures.

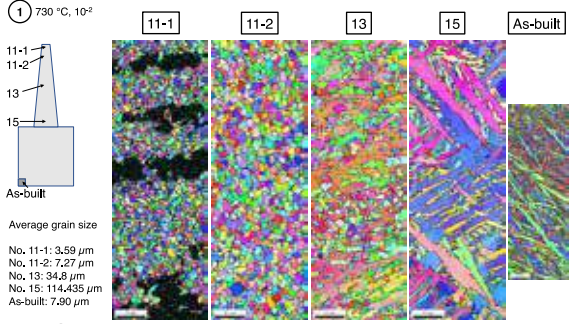

Fig.1 Grain evolution along the gauge length under as-fabricated conditions (EBSD: 730°C@10-2 (mm/mm)/s))

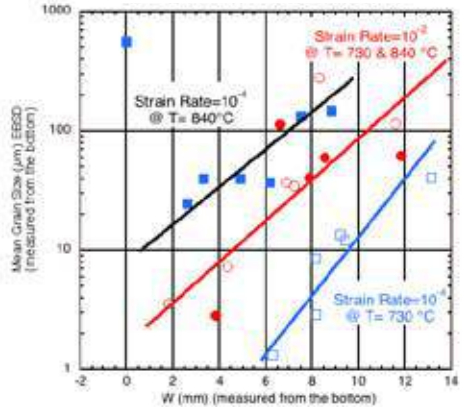

Fig.2 Evolution of the average grain size along the gauge length from the bottom to the fracture surface of the tested plate samples for both strain rates and temperatures.

Powders are indeed the essential raw materials for the new disruptive technology of ALM (3D manufacturing). These meetings allowed us to propose a tripartite scientific and technical research between Japan, France and Canada (3Countries) on joint international collaborations (named 3D3C) for the characterisation of powders obtained by different technologies.

Progress in the preparation of 3D3C

MR's unique and highly efficient characterisation facilities and powder production facilities in these countries are essential for the success of such an international collaboration. French industries such as Safran, Constellium and Addup have already expressed their interest. The "France Additive" association, which brings together all the players in additive manufacturing in France, is interested in this type of project. The Institut de Recherche Technologique Matériaux Métallurgie et Procédés (IRT-M2P) with the LEM3 laboratory has developed a machine for characterising the spread of powders that is much more representative than the current standardised tests. This laboratory will be contacted for this project. In collaboration with Professors Akihiko Chiba and Kenta Yamanaka and the IRT-M2P, we will carefully pursue the development of this project.

Keywords: Ti6Al4V, ALM, high temperature tensile test, EBSD

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Dynamical stability switching of a magnet by spin-orbit torques

We discovered a novel magnetic reversal process promoted by spin-orbit torque excitation. This can only be achieved by a specific energy landscape where we only have one local minimum in the classical analog of the Bloch sphere. We experimentally show the magnetization reversal using magnetoresistance and ferromagnetic resonance experiments, fully supporting an idea that the moments can be excited to point around the energy maximum upon large excitation.

Year 2022 would be the time where we started slowly building confidence that we can come out of the restricted life posed by the pandemic outbreak. I was one of those who were eager to feel the academic normality as was granted in the past and this visiting fellowship was spot-on for that. Personally, this is a special one since I was a student at Tohoku university a long time ago.

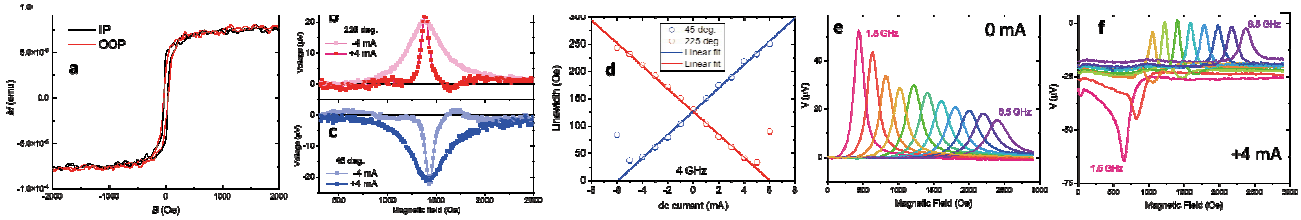
Within the field of spintronics, an efficient control of magnetization has been the central topic since its birth. This is due to its direct relevance to the majority of memory and logic applications based on the spin degree of freedom, where information is stored and processed using magnetic moments. In general, the non-volatility of magnetism, arising from magnetic anisotropies, is an essential component for spintronic memories and the community has devoted a great deal of efforts to achieve a large size of magnetic anisotropies in a spintronic memory cell, at the nanometer lengthscale. In this project, we consider the opposite side of this limit, namely making a magnet isotropic as much as we can and exploring new spintronic phenomena based on isotropic magnets. Magnetic Materials Lab at IMR has world-class capability of growing thin-films at an atomic level, an ideal place to pursue this ambitious project. During the period of this visiting professorship between July and August 2022, I was able to grew thin-films, optimized their magnetic properties, measured the patterned devices and analyzed the results, all by myself with Dr Seki. It reminded me my postdoc period a long time ago and I am very fortunate to have that back again, which was truly enjoyable.

We first grew multilayer stacks of MgO/ CoFeB/W on SiO_2/Si substrates. When we normally grow this type of stacks, the magnetic dipole interaction (often called the demagnetization) due to the thin-film nature is fully activated, creating the magnetically easy plane anisotropy. In order to counteract to this, which is essential to create a magnetic film with zero magnetic anisotropy, we employ the spin-orbit driven surface anisotropy. Therefore, the first task in this project was to find the optimal growth/annealing conditions that can level the surface anisotropy to the demagnetization. After growing more than ten different multi-layers and testing a number of annealing conditions during three weeks, we found conditions where hysteresis loops for in-plane and out-of-plane magnetic field directions almost match to each other as shown in Fig. 1a.

We then patterned a few of these multilayers to produce micro-bars for spin-torque excitation measurements. We extensively studied these micro-bars using microwave current excitation techniques and discovered that the magnetic relaxation, measured by the linewidth of magnetic resonance peaks, can be modified considerably by a dc current insertion, as shown in Fig. 1b&c. The Gilbert damping coefficient α represents the intrinsic magnetic relaxation and is extracted by the frequency dependence of linewidth. When we apply a dc current, spin-transfer torques are created due to the spin-Hall effect and modify α by following the phenomenological equation [1]:

$$\alpha = \frac{\sin\phi}{(H_{ext}+0.5M_{eff})\,\mu_0 M_s t}\frac{\hbar}{2e}\theta_{SH} J_c$$

Fig.1: **a** Magnetic hysteresis loops, in-plane (IP) and out-of-plane (OOP), for MgO/ CoFeB/W sample after optimization. **b&c** the ferromagnetic resonance peaks under dc current injections. **d** The linewidth as a function of dc excitation. **e&f** The frequency dependence of FMR peaks with and without dc excitation.



Here, μ_0, H_{ext}, M_{eff}, M_s, t, $\hbar$, e, θ_{SH} and J_c are the magnetic permeability of free-space, the externally applied magnetic field, the effective magnetisation, saturation magnetisation, the thickness of the magnetic layer, the reduced Planck constant, the elementary charge, the spin-Hall angle and the charge current density, respectively. The extracted θ_{SH} using this equation and the slope in Fig. 1d is 0.22 which is consistent with reported values in the literature [2]. We attribute the large damping modulation to the minimized M_{eff} in our devices. What is noticeable is that when the damping is fully compensated by injected spin transfer torques, we do observe the sign change of the FMR peak amplitude as shown in Fig. 1f, which is absent in the same experiments without dc current excitation (Fig. 1e). Phenomenologically, the FMR amplitude is determined by the phase relationship between the input microwave current and the dynamic component of magnetization precession (excited by the microwave current). The sign switching therefore means the π shift of the precessional phase, indicating the reversal of static magnetization.

To identify whether indeed the magnetization reversal is present or not, we performed magnetoresistance experiments with the spin-torque excitation. Figure 2a shows that there is a peak-like magnetoresistance only for the magnetic field direction when the spin-torques compensate the magnetic damping (so when we take the same set of data by reversing the magnetic field, this peak is absent).

The peak position represents the point where the intrinsic damping is fully compensated by the injected spin torques. We went on to analyse the peak position as a function of applied field direction/magnitude, as shown in Fig. 2b. The dependence excellently matches to the damping compensation model, e.g. the solid lines/curve are those calculated by the model.

Figures 2c&d would visually explain how the damping modulation leads to the magnetization reversal. The magnetization is equilibrated at the energy minimum defined by the Zeeman energy due to the applied magnetic field. What is interesting is that by applying anti-damping torques, the moments start to be excited away from the energy minimum and at high excitation, the time-averaging position of the moments can even be situated around the maximum of the energy landscape. The numerical simulations based on the stochastic Landau-Lifshitz-Gilbert equation capture the magnetization reversal phenomenon as shown in Fig. 2d where the color dots are used to relate the moment position with respect to energy potential in Fig. 2c.

Working with our theorists (Prof. Gerrit Bauer and Dr Yamamoto, JAEA), we are now developing an analytical model that can fully capture our observation. This study potentially offers a model system to explore the dynamical stability in spin systems and we are very fortunate to have had this visiting professorship opportunity that allowed this discovery.

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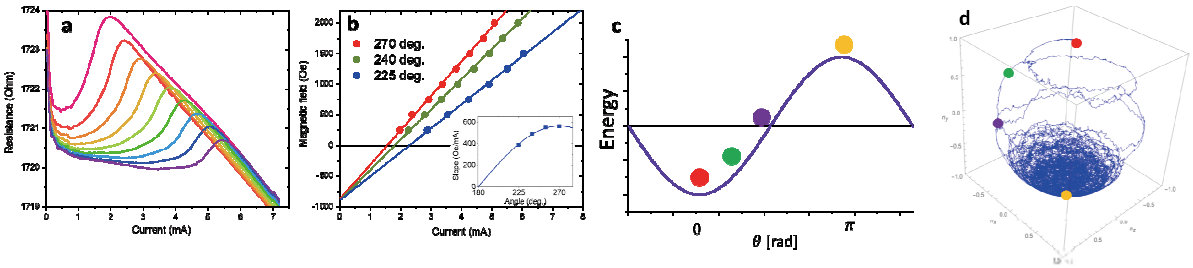

Fig.2: **a** Magnetoresistance under dc current excitation. **b** The peak analysis for different field amplitudes and directions. **c** A schematic of an energy landscape defined by the Zeeman energy. **d** A time-evolution of magnetic moments with a negative damping coefficient. A magnetic field is applied towards the north pole defined as θ = 0. Color dots are used for indicating corresponding states in the energy landscape in Fig 2c.

Keywords: spin current, spintronic, sputtering

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Guest Induced Spin-State Switching in Hoffmann-type Coordination Polymers

The reversible interconversion between the high-spin (HS) and low-spin (LS) states in transition metal complexes is being studied in the presence of different stimuli. The advantage of the porous Hoffmann-type framework is that the adsorption and desorption of gas molecules can play an important role in switching the spin state. The study of the guest-induced spin-crossover behavior of these materials is initiated in this short project.

Molecular magnetism, particularly spin-state switching in transition metal complexes[1], is a thriving field of research for its potential applications in memory devices, magnetic sensing etc[2-3]. For studying spin-state switching, the stimuli like light, pressure, and temperature are used for the 3d transition-based complexes and materials[4-5]. Interestingly gas-responsive spin-state switching is a unique field of research as a very-selected group of scientists can do it and need a high level of technical knowledge and scientific understanding. The Miyasaka group has the expertise in studying gas-responsive magnetic property changes in the framework materials and is credited globally with developing this area of research[6-8]. They also study the single-crystal to the single-crystal transformation of these materials using X-ray crystallography in the presence of different guest molecules, mainly gases and solvents as well. The group is globally known for the design of materials using redox-active ligands and [Ru_2] paddlewheel units as building blocks[6]. These special classes of complexes go through “gate opening” phenomena and are followed by structural changes that initiate the electron transfer between the metal and redox active ligand as well as a change in magnetic properties in the materials. On a different aspect, it is needless to mention that the extreme sensitivity of the spin-crossover(SCO) phenomenon to minute structural changes imposes a formidable challenge in designing SCO materials with targeted properties. In that context, Hofmann-type coordination polymers (HCPs) having the general formula $\{M(L)_n[M'(CN)_4\}$ or $[M(L)_n\{M''(CN)_2\}_2]$ where (M=Mn, Fe, Co, Cu, Zn or Cd, M′=Ni, Pd or Pt, M”=Ag or Au, L=pillar ligand) are of great interest[9], as the polymeric network exhibits stronger cooperativity between the SCO sites linked through covalent bonds to create a rigid lattice. Additionally, the organic linkers determine the shape and size of the framework and supramolecular interactions present in the solid state. Guest molecules inside the pores influence the cooperativity via weak interactions and create a pressure effect.

We have designed and synthesized a few crystalline Hoffmann frameworks by changing the organic linkers and the tretracyanometallates(Palladium and Platinum).

The complex we studied is a 2D framework with methyl isonicotinate acts as a pillar(pendant) ligand to form a 2D interdigitated structure[Fig. 1]. The complexes show different spin-state switching behavior in the presence and absence of solvent guest molecules in the pores[Fig. 2]. The complex retain its crystallinity after removal of the guest solvent molecules and the structure of the desolvated samples was also determined using X-ray crystallography[Fig 1]. The BET surface area measurement found that the framework of interest shows pressure-induced structural phase change and may have the potential to show gas-induced spin state switching behavior. The sample went through the initial screening, and the rest of the measurements will be done once a large amount of the sample would be prepared. During my visit, I also experienced the complex setup of gas-induced magnetic data collection that coupled a BET instrument with the MPMS5 magnetometer. The tubing, valves, and pressure gauges are assembled fascinatingly to obtain the results of the highest authenticity.

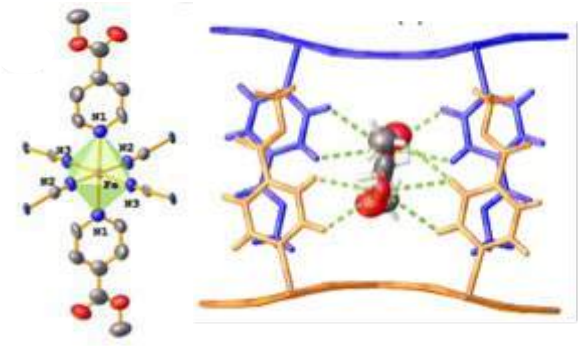

Fig 1. Asymmetric unit of $[Fe^{II}(L)_2Pd(CN)_4]\cdot 1.3MeOH$ (L = methyl isonicotinate), and position solvent molecules in between the layers.

The complex experimental setup to collect the single crystal X-ray data of the porous frameworks under a positive pressure of a gas is very challenging and an excellent experience for learning. Also, in this case, the gas pressure of the capillary containing the crystal is controlled by a BET instrument. Some of the magnetic materials we design are porous, highly stable, and suitable for studying their gas-responsive

magnetic properties as well as structural changes in the presence and absence of guest gas molecules.

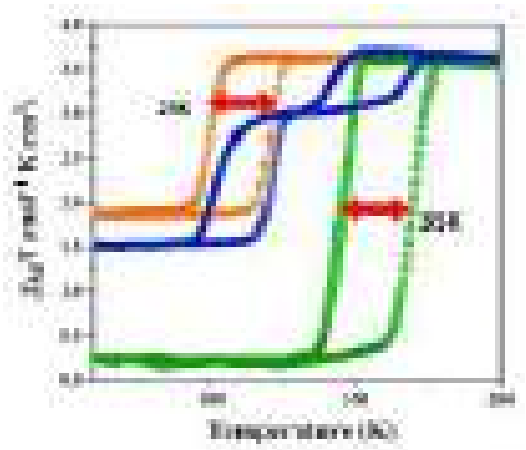

Fig. 2. Variable temperature magnetic susceptibility plot of Fe(4-acetyl pyridine)2[Pd(CN)4])·1.5 MeOH (1·1.5MeOH), (solvated: orange), 1·0.4MeOH (partial desolvated:blue) and 1 (Complete desolvated: green).

Overall, the work initiated during my stay at ICC-IMR is very much collaborative in nature and will need further experiments to conclude. We look forward to completing all the experiments and characterization to write a paper together, where ICC-IMR will be acknowdgeled with due credits.

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Keywords: Magnetic Properties, Crystals
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3D Atom Probe (3DAP) Studies in a Ti-6wt%Mo Alloy

Abstract

3D atom probe (3DAP) studies were conducted in a Ti-6wt%Mo model alloy to quantify Mo concentration across the hcp-bcc interface. Further, the interaction of alloying elements with interfaces was discussed for gain boundary segregation of C and P in iron model alloys.

As part of my Sabbatical I was as a Visiting Professor at IMR in the group of Professor Tadashi Furuhara from July 11 to September 12, 2022. My local host was primarily Professor Goro Miyamoto. The research stay was motivated by our joint research interests on the role of alloying elements on migrating interfaces in metallic systems, in particular steels and titanium alloys. My research emphasizes primarily steels but one of my recent PhD students, Mariana Rodrigues, studied phase transformations in titanium alloys which have a number of similarities to phase transformations in steels. The laboratory of Professor Furuhara has also particular expertise on titanium alloys and we were able to facilitate a research visit of Mariana at the IMR in 2019 where she initiated 3D atom probe (3DAP) studies in a Ti-6wt%Mo model alloy to quantify the interaction of Mo with the hcp-bcc interface during phase transformations in this alloy. Mo is an important alloying element in many industrial Ti alloys that stabilizes the bcc-phase, i.e. Ti alloys with dual phase bcc-hcp microstructures can be created with unique properties for aerospace and biomedical applications. The progress of these 3DAP studies was affected by the COVID pandemic and my research visit was designed to revitalize the 3DAP studies. We prepared at the University of British Columbia (UBC) a number of different Ti-6wt%Mo samples that had undergone different heat treatment scenarios. These samples were then prepared at IMR for the SEM/EDS and 3DAP studies that confirmed redistribution of Mo from the hcp (α) phase into the bcc (β) phase as well as an enrichment of Mo at the hcp-bcc interface, as shown in Figures 1 and 2. Mo partitioning and enrichment at the interface were characterized with respect to interface coherency, namely a presence of Burgers orientation relationship. Doing repeat measurements we were able to reproduce quantitatively the enrichment levels of Mo for the investigated heat treatment conditions. Further, we found that the Mo enrichment appears to be insensitive to the interface character, i.e. Burgers vs Non-Burgers crystallographic orientations. As

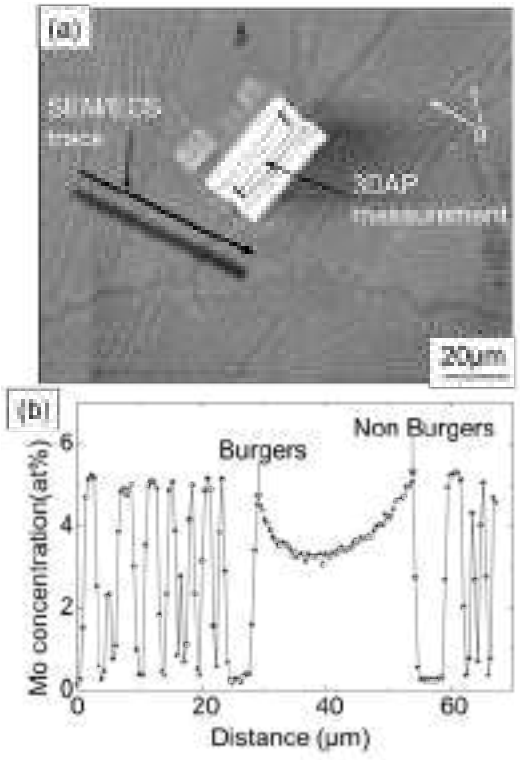

Fig. 1: (a)SEM images showing (α+β) microstructure and the locations for SEM/EDS and 3DAP measurement, (b) Mo concentration profile in the Ti-6wt%Mo alloy heat treated at 800 °C for 3 hours.

a result of my research visit we have meanwhile completed these 3DAP studies and are in the process of preparing a brief manuscript for a referred journal publication.

My research stay provided also an excellent opportunity to discuss individual research projects of faculty members, postdoctoral fellows and graduate students in the laboratory. In particular we discussed 3DAP results in Fe-model alloys where C and P grain boundary segregation was observed. For the quantitative analysis of these results we reviewed the role of the interface thickness that is somewhat obscured, in part, due to experimental broadening of segregation profiles. We emphasized that the interfacial excess is the relevant quantity,

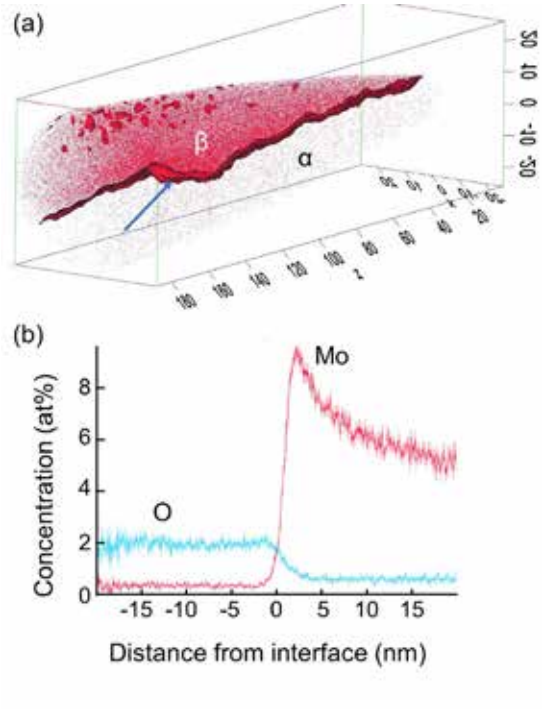

Fig. 2: (a)three-dimensional Mo atom maps, (b) Mo and O concentration profiles across bcc/hcp interface obtained with 3DAP in the Ti-6wt%Mo alloy heat treated at 800 °C for 3 hours. The isosurface of 3at% Mo is shown.

i.e. the projection of excess solute concentration per unit interfacial area. This approach is consistent with a multi-scale modelling analysis of solute drag in my group at UBC that we had proposed by analyzing experimental data on grain boundary motion during recrystallization of pure gold containing Bi and Fe impurities at the ppm-level [1]. With a seminar talk entitled "Interface-based Alloy Design – A New Frontier to Engineer Microstructures" I provided an overview on these research areas in my group at UBC.

Further, I was able with the assistance of IMR to have in the period August 28 – September 1 brief visits to two steel companies, i.e. Nippon Steel and JFE, as well as the Tokyo University of Agriculture and Technology (Professor Yamanaka) and the Tokyo Institute for Technology (Professor Nakada). These visits were designed to exchange and discuss research topics related to ferrous metallurgy and computational materials science. I gave the following three lectures during these visits:

1. Interface-based Steel Design, Nippon Steel, Kimitsu.
2. Modelling of Microstructure Evolution, Tokyo University of Agriculture and Technology, Tokyo.
3. Microstructure Design of Advanced High Performance Steels, JFE, Chiba.

References

[1] A. Suhane et al., Acta Mater, 224, 117473 (2022)

Keywords: Phase transformation

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Group photo with Prof. Furuhara Group together with other ICC-IMR visitors (2022.9.8)

Kinetic behavior of solid-liquid interface during Si solidification from the melt

In situ observation of silicon solidification from the melt has shown that the facets, formerly expected to grow by 2D nucleation kinetic, are in fact surfaces vicinal to (111) facets. The variable terrace length is expected to depend on the facet-rough interface angle. The effect of the interaction of single dislocations with the vicinal facets is also described.

For two decades now, the IMR Tohoku is performing in situ measurements and visualization of the solid-liquid interface during solidification of metals and semiconductors, especially silicon. In parallel, more than 10 years ago, the group in Grenoble published a series of theoretical papers on the kinetics of grain boundaries in the growth of silicon from the melt. These papers predicted that a groove, constituted by (111) facets, should exist at the grain boundary-growth interface triple line.

The experimental results obtained in Sendai indeed showed that these facets and groove exist during silicon growth. The purpose of this two month visit, from 1st October to 30th November 2022, was to confront experiment and theory, for a better understanding of the grain boundary behavior during silicon growth.

During three one-hour seminars, I presented our understanding of Si kinetics, including dislocation behavior and twinning during growth. After discussions with all the researchers of Fujiwara laboratory, I more precisely focused my attention on the experimental results of two students working on their PhD, both with in-situ recording of Si growth. Shashank Mishra was using pre-oriented seeds in order to observe perfectly defined grain boundaries. Fan Wang on the contrary did not used seeds, so that she observed totally random grain boundaries.

A first step has been to determine the temperature gradient at the solid-liquid interface. As it was not possible to measure it precisely during the experiments, I developed a linear approximation of the heat flux in the sample, giving simultaneously the variation of growth rate and of temperature gradients (in liquid and solid) with time. As can be seen on the Figure 1, the agreement of the model with the measured growth rate was good and then the temperature gradients were reliable.

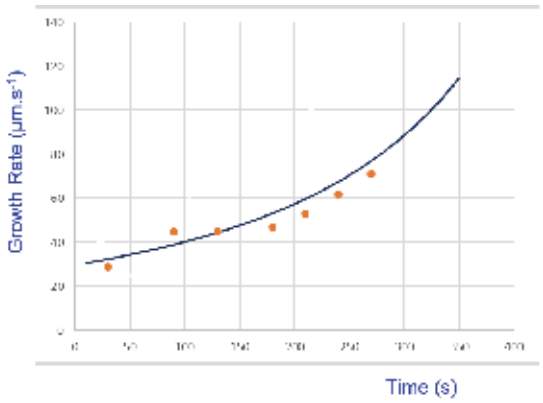

Fig. 1 shows the growth rate of a solid-liquid interface as function of time. The experimental results (orange dots), fit well with the theoretical calculation (blue line).

From these calculated temperature gradients, it was possible to measure the undercooling of the grain boundary grooves and of the growing facets.

In Shashank's experiments, thanks to the well oriented grains, it was possible to observe facets growing perpendicularly to the temperature gradient. It appeared immediately that the relationship between the growth rate and the undercooling of facets did not fit at all, neither with a 2D-nucleation growth law, neither with a dislocation-driven growth model. We finely concluded that the observed facets were indeed surfaces vicinal to (111) facets, growing through a terrace-step mechanism [1]. In order to better explain the results, we added the hypothesis that the terrace length depends on the angle between the vicinal surface and the rough solid-liquid interface.

Another result of these experiments was the angle measured between the grain boundary and the growth direction, in the case where no groove was observed. From this angle it has been possible to propose a ratio between the kinetic coefficients of the (100) and (110) oriented solid-liquid interfaces [2].

Concerning Fan's experiments, she observed large grooves at the grain boundary intersection with the solid-liquid interface. Here also, the measured undercooling did not fit to 2D-nuclation and vicinal surface growth kinetic was also concluded. From time to time a strange behavior occurred, leading to decrease and increase of the groove size and facet velocities. This phenomenon was explained by the periodic interaction with single dislocations impacting the facet kinetics [3]. Figure two shows an experimental picture of the groove variations and the results of a geometrical model that we developed on the basis of the dislocation interaction.

Fig. 2, shows the experimental observation of a grain boundary groove interacting with dislocations and the geometrical simulation of the kinetic mechanisms involved in these interactions.

In other experiments, it was observed that sometimes dislocations can pass through a twin during solidification, while in most experiments, they are blocked at the boundary. A model has been developed taking into account the possible continuity of gliding planes from one grain to the other through the twin boundary. It was shown that dislocations can glide along three common planes in the case of a Σ3 twin and along one common plane only in the case of a Σ9 twin.

In a final seminar, I presented to the laboratory a summary of our results and a number of recommendations for future work in the group, including the interest of numerical simulation for a better understanding of the experiments, and a series of experiments to perform in order to investigate more quantitatively the phenomena that we observed.

In conclusion, I would like to thank very much the institute for Materials Research of Tohoku University and Professor K. Fujiwara for this invitation to participate to this fascinating research program. Thanks to the excellent experimental work performed in this unit, we have been able to explain the kinetic behavior of the silicon facets and show that vicinal facet growth also exists in solidification and crystal growth from the melt. To the best of our knowledge, it is the first time that vicinal growth is demonstrated in the case of crystal growth from the melt.

References

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Shashank Shekhar Mishra, Lu-Chung Chuang, Nozawa Jun, Kensaku Maeda, Haruhiko Morito, Thierry Duffar, Kozo Fujiwara
Poster presentation, ICCGE-19, July 30-August 4, 2023, Napoli, Italy
Paper for Scripta Materialia in progress

[2] "Growth behaviors at crystal melt interface at {100}, {110} and {111} planes of silicon during unidirectional solidification"
Shashank Shekhar Mishra, Lu-Chung Chuang, Nozawa Jun, Kensaku Maeda, Haruhiko Morito, Thierry Duffar, Kozo Fujiwara
ICCGE-19, July 30-August 4, 2023, Napoli, Italy
Paper for J. Crystal Growth in progress

[3] "Dislocation interaction with facet groove at silicon grain boundary"
Yang Fan, Lu-Chung Chang, Kensaku Maeda, Jun Nozawa, Haruhiko Morito, Kozo Fujiwara, Thierry Duffar
Oral presentation ICCGE-19, July 30-August 4, 2023, Napoli, Italy
Paper for J. Crystal Growth in progress

Keywords: directional solidification, kinetics, grain boundaries
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Crystal Growth of Differently Doped Mixed Oxides Compounds of Perovskite, Garnet and Olivine Structures

The crystals of $YAlO_3$ (YAP) $Y_3Al_5O_{12}$ (YAG) and $LiMgPO_4$ (LMP) differently doped with rare-earth (RE) elements were investigated within this work. The crystals were grown from the melt using micro pulling-down method at the Research Laboratory on Advanced Crystal Engineering, Yoshikawa Laboratory, Tohoku University, Sendai, Japan. Luminescence and energy–storage properties of the obtained crystals were studied at the Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland using different spectroscopic methods.

The RE-doped LMP compound is nowadays considered as very promising dosimetric material, as its luminescent properties are comparable or in a few aspects even better as compared to LiF or Al_2O_3.

In turn, the RE-doped YAP and YAG are rather known as fast and efficient scintillators and thus the investigation of the energy-storage properties of such materials remains rarely seen. Therefore, within this work, we want to indicate that the RE-doped YAP perovskite can be also applied as very promising energy-storage phosphor for dosimetric applications. This topic is also very actual nowadays because the evidence of energy-storage by mixed oxides compounds of perovskite and garnet structures was recently reported by our research group from Krakow. Moreover, the infra-red stimulated luminescence (IRSL) emission in Ce^{3+} doped YAP, YAG and $Lu_3Al_5O_{12}$ (LuAG) crystals was also investigated [1-3].

The investigated crystals were grown from the melt by the micro pulling-down (MPD) method. The detailed description of this method can be found in our previously published papers [1-3]. The luminescence properties were investigated by different spectroscopic techniques, such as Thermoluminescence (TL(T)), TL(λ) spectral measurements, the Infra-red-light stimulated luminescence (IRSL) and Cathodoluminescence (CL).

For TL measurements the semiautomatic Risø reader model TL/OSL-DA-20 has been utilized. The reader is equipped with $^{90}Sr/^{90}Y$ beta source and ^{241}Am alpha particle source that were used for samples irradiations. All samples were read out with the same temperature regime, namely from room temperature (RT) to 400 ^oC at the constant heating rate of 2 $^oC/s$.

For spectrally resolved TL(λ) measurements, a high-sensitive Ocean Optics QE PRO grating spectrometer was connected to the Risø reader instead of the standard photomultiplier tube. This device allows to record luminescence emission in the range from 200 to 1000 nm with a 4 nm resolution. The signal is delivered from the sample to the spectrometer via optical fiber of a core diameter of 400 μm. Its flat spectral characteristic causes that the measurements can be done without any additional optical filter. Therefore, the measured data are not affected by the spectral characteristics of the applied photomultiplier and optical filters as it is in the case of the measurements performed with the standard reader. On the other hand it should be noted, that sensitivity of the spectrometer is much lower than that of the photomultiplier.

Fig. 1 shows the studied crystals: $YAlO_3$ (panel A), $Y_3Al_5O_{12}$:Ce (panel B) and $LiMgPO_4$:Tb,B (panel C).

CL measurements were done in cooperation with the Institute of Physics Kazimierz Wielki University in Bydgoszcz, Poland. The CL spectra were measured at RT using 10 keV electron

beam excitation from electron microscope SEM JEOL coupled with a Stellar Net grating spectrometer with TE-cooled CCD detector working in the 200–1100 nm range with a 1 nm resolution. It should be mentioned that e-beam excited CL and X-ray excited RL well imitate scintillation phenomena in the crystals under study. It is worth noting that 10 keV electrons are unable to produce new host defect centers due to high displacement energy for knock-out mechanisms in binary and complex oxide.

We have also checked the different preheating temperatures before the IRSL measurements to correlate the signals measured using TL and IRSL phenomena for investigated the obtained YAP crystals. The results are shown in Fig. 2 (left). Fig. 2 (right) shows the differences in the IRSL emission intensities for YAG:Ce crystals of different Ce^{3+} concentration.

It was also shown that the IR stimulation mostly affects the low-temperature peak (100-160 ◦C) while the high-temperature peaks remain less affected. Finally, due to highest radio-sensitivity and lowest fading, we concluded that both YAG and YAP crystals seem promising for dosimetric applications.

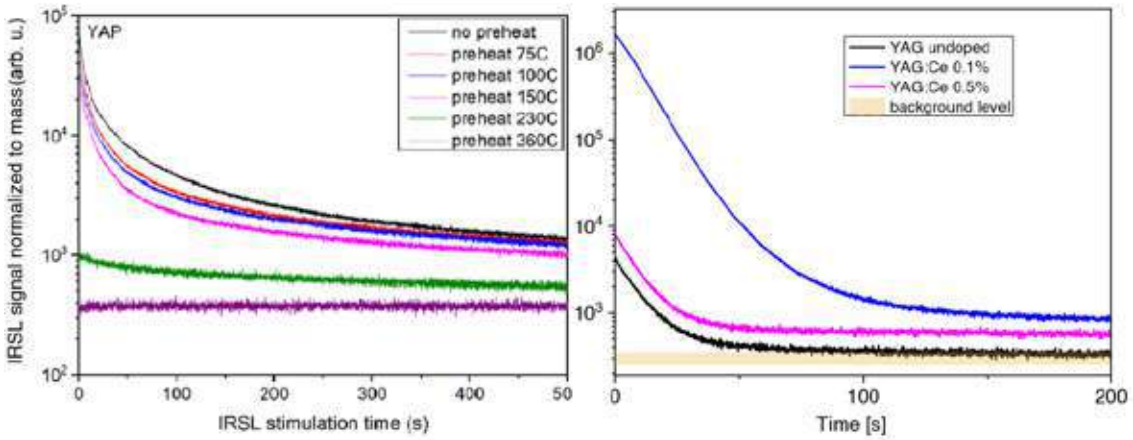

Fig 2. Comparison of the IRSL signals measured for YAP investigated samples (panel left) and YAG investigated samples (panel right)

Keywords: crystal, crystal growth, Czochralski growth
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[2] P. Bilski, A. Mrozik, W. Gieszczyk, S. Nizhankovskiy, Yu. Zorenko. Infrared Stimulated Luminescence of Ce^{3+} Doped YAG Crystals. Materials 15 (2022), 8288

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Activity Report

Workshops

Workshops

No.	Chairperson or Committee Member	Title of Workshop	Place	Term
22WS01	Prof. Miyasaka	IMR International Workshop on Frontier and Perspectives of Molecule-Based Magnets	Sendai	2022.10.8-10.11
22WS02	Prof. Tsukazaki	29th International Conference on Low Temperature Physics	Sapporo	2022.8.18-8.24
22WS03	Prof. Kato	17th International Workshop on Biomaterials in Interface Science	Sendai	2022.8.24
22WS04	Prof. Aoki	International Workshop on Novel Superconducting and Topological Phenomena of UTe2 and Related Materials	Sendai	2023.11.30-12.2
22WS05	Prof. Nojiri	Asia-Pacific Conference on Condensed Matter Physics 2022	Hybrid, Sendai	2022.11.21-11.23
22WS06	Prof. Aoki	Recent Topics in Low Temperature Physics	Sendai	2022.8.17
22WS07	Prof. Sasaki	The 6th Symposium for the Core Research Clusters for Materials Science and Spintronics, and the 5th Symposium on International Joint Graduate Programs in Materials Science	Online	2022.10.24-11.27
22WS08	Prof. Yoshikawa	International Symposium on Functional Materials 2022 Autumn Seminar	Sendai	2022.10.29-10.30
22WS09	Prof. Awaji	7th French-Japanese High Field & HTS Magnet Technology Research Collaboration Workshop	Sendai and Zao in Yamagata	2023.3.8-3.10

IMR International Symposium 2022 on Frontier and Perspectives of Molecule-Based Magnets

研究代表者：東北大金研 宮坂 等 [1]
研究分担者：東北大院理 山下 正廣 [2]

IMR International Symposium 2022 on Frontier and Perspectives of Molecule-Based Magnets
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Keywords: molecule-based magnet, molecular magnetic materials, IMR international workshop

Molecule-based magnets and their related materials have been attracted much attention from the viewpoint of their designability, tunability, lightness, transparency, etc., compared with those of the conventional metal-based magnets. Molecular magnetic materials are possible to take a variety of structural lattice dimensionality from discrete to three-dimensional form, and exhibit intriguing properties associated with nano-sized quantum magnetic phenomena and spin-crossover, and stimuli-sensitive magnetic properties, etc. With the support of Yamada foundation, we held IMR international Symposium 2022 and 73th Yamada Conference in the term of 8–11 October, 2022, in which we discussed the frontier and perspectives of the molecule-based magnets and molecular spintronics.

1. 緒言

分子磁性体は、今日、分子性の機能性物質の代表格の一つとして世界の第一線で研究されている。ボトムアップ的に設計・合成される分子磁性体やその関連物質は、孤立系分子やクラスター、一次元鎖、二次元層状構造などの低次元系から三次元無限格子まで、構造的な観点から眺めても様々に展開される。最近では、単分子磁石や単イオン磁石、そして表面での単分子アプローチに代表されるような量子物性への興味や、金属—有機骨格体（Metal-Organic Framework; MOF）の多孔性に着目した磁気相の化学外場応答などのバルク物性制御に至るまで、新しい物質や分子材料の開発に加え、新しい現象やアプローチが幅広く精力的に研究されている。また、この分野は近年様々な分野との複合領域を形成しており、今後益々重要な分野を形成していくと考えられる。今回、理学研究科化学専攻の山下正廣名誉教授と共同で分子磁性のシンポジウムを計画し、山田科学振興財団から財政的なサポートを受けることにより、「第 73 回山田コンファレンス」と合同で金研国際シンポジウムを開催することになった：The 73rd Yamada Conference and Institute for Materials Research International Symposium 2022。開催日程は、2022 年 10 月 8-11 日の 4 日間である。このうち、10 月 8 日の朝から夕方を「金研国際シンポジウム 2022」と位置づけて、分子磁性体とその機能制御や高温分子磁性体に焦点を当て、後の 8 日のイブニングセッションから 9–11 日を「第 73 回山田コンファレンス」として、単分子磁石や単イオン磁石、分子磁石の量子性やスピントロニクスについての話題を中心に議論した。

2. 開催内容

金研国際シンポジウム 2022 と第 73 回山田コンファレンス、合わせて 12 ヶ国 108 名の参加者を数えた。COVID-19 の影響により多くの中国の研究者はオンライン参加であったが、12 ヶ国の内訳は、日本 (80 名)、英国 (1 名)、ドイツ (3 名)、中国 (6 名)、スペイン (3 名)、フランス (4 名)、米国 (4 名)、ポルトガル (1 名)、イタリア (2 名)、カナダ (2 名)、ポーランド (1 名)、ルーマニア (1 名) であった。このうち、世界の第一線で活躍する 45 名の研究者（中国を除く海外の研究者全員）を招待し、最近のホットな話題について質疑応答時間を無制限として議論した。また、初日の金研国際シンポジウムでは、午後を Raising Star Session として、国内外の 4 名の若手研究者に講演をお願いした。ちなみに、本会議の開催時はまさに COVID-19 の影響により海外渡航が制限され、

それがちょうど緩和された時期であったため、オンサイト face-to-face で自由に討論ができることに皆飢えていたということもあり、議論が非常に活発であったことが実に印象的であった。下記にプログラムと参加者の写真を掲載する。詳細は下記 URL を参照 ：https://sites.google.com/view/yamada-conference73/home

The 73rd Yamada Conference and Institute for Materials Research International Symposium 2022

Institute for Materials Research International Symposium 2022 (Venue: Sakura Hall, Tohoku University) **8th in October 2022**		
8:55 ~ 9:00	Hitoshi Miyasaka (Tohoku University, Japan)	Opening for IMR International Symposium2022
9:00 ~ 9:30	Yuko Hosokoshi (Osaka Metropolitan University, Japan)	“Quantum states in frustrated molecular magnets”
9:30 ~ 10:00	Corine Mathonière (University of Bordeaux, France)	“Switchable compounds: Charge transfer or spin crossover ?”
10:00 ~ 10:30	Masaaki Ohba (Kyushu University, Japan)	“Multi-step spin transition in a Hofmann-type clathrate”
10:30 ~ 11:00	Coffee Break	
11:00 ~ 11:30	Rodolphe Clérac (University of Bordeaux, France)	“New room temperature metal-organic magnets”
11:30 ~ 12:00	Kathryn Preuss (University of Guelph, Canada)	“Magnetic ordering in metal-radical complexes”
12:00 ~ 12:30	Yasutaka Kitagawa (Osaka University, Japan)	“A quantum chemical approach to magnetic molecules and its application”
12:30 ~ 13:30	Lunch + Poster Session Preparation	
13:30 ~ 14:00	Tetsuro Kusamoto (Institute for Molecular Science, Japan)	“Spin-correlated photofunctions based on luminescent radicals” (Rising Star Session)
14:00 ~ 14:30	Zhao-Yang Li (Nankai University, China)	“Hyperfine switching of spin crossover through precise chemical doping” (Rising Star Session)
14:30 ~ 15:00	Leoni Barrios (University of Barcelona, Spain)	“New supramolecular architectures combining spin crossover, single ion magnet and quantum coherence properties” (Rising Star Session)
15:00 ~ 15:30	Yoji Horii (Nara Women`s University)	“Two-dimensional MOFs composed of single-molecule magnets“(Rising Star Session)
15:30 ~ 15:35	Hitoshi Miyasaka (Tohoku University, Japan)	Closing for IMR International Symposium2022
The 73rd Yamada Conference (Venue: Sakura Hall, Tohoku University) **8th in October 2022**		
15:35 ~ 16:05	Coffee Break	
16:05 ~ 16:30	Yoshio Kitaoka (Osaka University, Japan)	Opening Ceremony-1
	Masahiro Yamashita (Tohoku University, Japan)	Opening Ceremony-2
16:30 ~ 17:00	Guillem Aromi (University of Barcelona, Spain)	“Heterometallic lanthanide complexes for quantum technologies”
17:00 ~ 17:30	Tadahiro Komeda (Tohoku University, Japan)	“Spin state of single molecule magnet contacted with superconductor surface for quantum information process”
17:30 ~ 18:00	J. v. Slageren (University of Stuttgart, Germany)	“Molecular spintronics: From strong coupling to electrical readout”
The 73rd Yamada Conference (Venue: Sakura Hall, Tohoku University) **9th in October 2022**		
9:00 ~ 9:30	Kazunobu Sato (Osaka Metropolitan University, Japan)	“AWG-based ESR as spin manipulation technology for molecular spin qubits”
9:30 ~ 10:00	Stephen Hill (NHMFL, USA)	“Application of wideband pulsed high-frequency EPR to molecular quantum spin science”
10:00 ~ 10:30	Roberta Sessoli (University of Firenze, Italy)	“The challenge of spin control with electric fields”
10:30 ~ 11:00	Coffee Break	
11:00 ~ 11:30	Eugenio Coronado (University of Valencia, Spain)	“Spin control in smart spintronic devices based on spin crossover complexes and molecular spin qubits”
11:30 ~ 12:00	Talal Mallah (Université Paris-Sud 11, France)	“Transition metal containing molecular magnets for quantum information”
12:00 ~ 12:30	ShangDa Jiang (South China University of Technology, China)	“Geometrical phase in the high spin magnetic molecules”
12:30 ~ 13:00	Lunch	
13:00 ~ 14:00	Poster Session	
14:00 ~ 14:30	Marius Andruh (University of Bucharest, Romania)	“Metal-radical complexes for spin qubits and single molecule magnets”
14:30 ~ 15:00	Valentin Alek Dediu (CNR-ISMM, Italy)	“Hybrid molecular-ferromagnetic interfaces - Towards radically new magnetic materials”
15:00 ~ 15:30	Hiroko Tokoro (University of Tsukuba, Japan)	“Correlation between the phonon frequency and long-range magnetic ordering on molecule-based magnets”
15:30 ~ 16:00	Coffee Break	
16:00 ~ 16:30	Richard Layfield (University of Sussex, UK)	“The metallocene paradigm in single-molecule magnetism”
16:30 ~ 17:00	Ming-Liang Tong (Sun Yat-Sen University, China)	“Building-block approaches to high-performance d-f single-molecule magnets”
17:00 ~ 17:30	Muralee Murugesu (University of Ottawa, Canada)	“Achieving strong magnetic coupling in lanthanide single molecule magnets”

17:30 ~ 18:00	Selvan Demir (Michigan State University, USA)	"Employing new radical ligands in lanthanide single-molecule magnets"
The 73rd Yamada Conference (Venue: Sakura Hall, Tohoku University) **10th in October 2022**		
9:00 ~ 9:30	Osamu Sato (Kyushu University, Japan)	"Polarization and magnetization switching via charge transfer in molecular crystals"
9:30 ~ 10:00	Vincent Repain (University Paris Diderot, France)	"Addressing single spin-crossover molecules in high density networks on surfaces"
10:00 ~ 10:30	Shinya Hayami (Kumamoto University, Japan)	"Ferroelectric SCO materials"
10:30 ~ 11:00	Coffee Break	
11:00 ~ 11:30	Tao Liu (Dalian University of Technology, China)	"Switching multi-functions utilizing spin crossover"
11:30 ~ 12:00	Manuel Almeida (University of Lisbon, Portugal)	"Development of molecular conducting and magnetic bilayers systems"
12:00 ~ 12:30	Lunch	
12:30 ~ 13:30	Poster Session	
13:30 ~ 14:00	Barbara Sieklucka (Jagiellonian University, Poland)	"Octacyanidometallates for multifunctional molecular materials"
14:00 ~ 14:30	Joel Miller (University of Utah, USA)	"Organic-based antiferromagnets"
14:30 ~ 15:00	Bin Hu (University of Tennessee, USA)	"Orbit-orbit interaction effects on optical properties in 2D perovskites"
15:00 ~ 15:30	Coffee Break	
15:30 ~ 16:00	Song Gao (Sun Yat-Sen University, China)	"Molecular spin state manipulation and spin chemistry"
16:00 ~ 16:30	Alexey A. Popov (Dresden, Germany)	"Surface magnetism in fullerene single-molecule magnets with lanthanide-lanthanide bonds"
16:30 ~ 17:00	Hirokazu Tada (Osaka University, Japan)	"Magnetoresistance in single molecules and molecular aggregates"
17:00 ~ 17:30	Takayoshi Nakamura (Hokkaido University, Japan)	"Supramolecular approach to multifunctional materials"
18:00 ~ 20:00	Banquet	Westin Hotel Sendai; "Miyabi" at 25th floor
The 73rd Yamada Conference (Venue: Sakura Hall, Tohoku University) **11th in October 2022**		
9:00 ~ 9:30	Hitoshi Miyasaka (Tohoku University, Japan)	"Manipulation of charge and spin in metal-organic frameworks"
9:30 ~ 10:00	Mario Ruben (KIT, Germany)	"Coherent spin-photon interfaces for quantum gates"
10:00 ~ 10:30	Katsuya Inoue (Hiroshima University, Japan)	"Coherent spin-phase long range order in chiral magnets"
10:30 ~ 11:00	Coffee Break	
11:00 ~ 11:30	Yan-Zhen Zheng (Xi`an Jiaotong University, China)	"Pushing the limit of lanthanide single-molecule magnets"
11:30 ~ 12:00	Masahiro Yamashita (Tohoku University, Japan)	"Molecular spin qubits and highly density memory devices based on molecular magnets"
12:00 ~ 12:10	Tadahiro Komeda (Tohoku University, Japan)	Closing Ceremony + Poster Award Ceremony
	Masahiro Yamashita (Tohoku University, Japan)	Closing Ceremony

4. まとめ

本会議は分子磁性やその関連分野の第一線で活躍する多くの研究者が集う機会となり、また COVID-19 の影響から若干落ち着きを取り戻してきた谷間のような時期（第 7 波と 8 波の間）にちょうど行われた。オンサイトでこのような国際会議を開催できたことを嬉しく思うし、久々に有意義で白熱した議論を楽しめたことが何よりもよかったと思っている。講演していただいた方々、参加していただいた方々には深く感謝したい。実際、本会議の計画は、2019 年に山下名誉教授と宮坂の間で計画され、本来であれば、2020 年には開催予定であった。COVID-19 の影響で 2 年間もズレてしまった訳である。本来であれば、国内外の研究者に金研に来てもらい、今後の共同研究の場として活用してもらうための周知の場としたいところであったが、残念ながら、COVID-19 の影響により金研の立ち入りが強く制限されていた時期であったため、どなたも金研に呼べなかったことが残念な点である。しかし、数年を待ってようやく開催した対面での国際会議を誰もが待ち望んでいたため、非常に活発で学問・分野の活性のみならず、研究者や参加した学生の活力を高めるといった意味でも極めて有意義な会議となった。最後に、本会議の関連で COVID-19 への感染がなかったことも報告したい。

謝辞

本会議の助成サポートをして頂いた金研 GIMRT および山田科学振興財団に感謝したい。また、本会議の運営を助けて頂いた本学大学院理学研究科化学専攻の錯体化学研究室、高石准教授グループ、山下名誉教授のグループ、多元物質科学研究所の米田研の皆さま、芥川研の皆さま、そして金研宮坂研の皆さまにこの場を借りて深く感謝申し上げたい。

Session sponsor for [Special Symposium: The 50th Anniversary of superfluid Helium 3] in 29th International Conference on Low Temperature Physics, 2022. 8. 18 - 24.

At 29th International Conference on Low Temperature Physics, Sapporo Hybrid format, 2022. 8. 18 – 24, a special symposium "The 50th Anniversary of superfluid Helium 3" was sponsored by Institute for Materials Research (IMR), Tohoku University. In this special symposium, Physics of Superfluid Helium 3 -Past, Present, and Future- was discussed with four invited talks. Two Nobel-prize laureates, Profs. Lee and Leggett delivered a historical story from the discovery.

The 29th International Conference on Low Temperature Physics (LT29) is a major meeting of the C5 Committee of the International Union of Pure and Applied Physics (IUPAP). It was held at the Sapporo Convention Center for 7 days from August 18th (Thursday) to 24th (Wednesday), 2022. Due to the pandemic caused by the new coronavirus COVID-19, the originally planned August 2020 event was not possible, and two years later it was held in a hybrid format. It was managed to hold the event after taking unprecedented measures such as to prevent infectious diseases, support for on-site as well as remote participation, and visa acquisition assistance for overseas participants. The number of on-site participants reached above 860 including 340 from overseas. In total, more than 1100 participants enjoyed lively scientific discussion.

The conference sessions focus on five sub-fields (1. Quantum Gases, Fluids and Solids, 2. Superconductivity, 3. Magnetism and Quantum Phases, 4. Nanophysics and Quantum Information, 5. Cryogenic Techniques and Device Applications). 2022 marks the 50th anniversary of the discovery of superfluid Helium-3. To celebrate this memorial year, the special symposium was held in LT29. Original logo (Fig. 1) was shown at the top page of LT29 website. Two Nobel laureates gave lectures at the special symposium. In addition to the scientific sessions based on the researchers, public lecture was also held online regarding the two interesting topics about superconductivity and quantum computing.

The superfluid ^{3}He was discovered in 1972. Superfluid ^{3}He was the first observed anisotropic superfluid and is still being actively studied. At LT29, a Special Symposium was held (Fig. 2): Physics of Superfluid Helium 3 -Past, Present, and Future with four invited talks. First, Prof. Bill Halperin, the chair of this session, talked about the significance of this symposium and the situation at Cornell University at the time of the discovery of superfluid ^{3}He. Two Nobel laureates, Profs. Lee and Leggett, then reported on the experimental and theoretical state of affairs before and after the discovery. Prof. Saunders reported on current and future research on ^{3}He. Many attendees at the main Hall learned their experiences and interesting physics on ^{3}He (Fig. 3).

As a session sponsor, IMR logo was shown on the LT29 website and the program booklet. The sponsor's contribution for this special symposium was recognized by the participants who are in the research field of low temperature physics. We are pleased with the success of this special symposium and entire conference programs.

References

[1] https://www.lt29.jp/

Fig. 1 A Logo for the 50th Anniversary of Superfluid Helium-3.

Keywords: Superconducting, magnetism,
Atsushi Tsukazaki (Low temperature physics division)
E-mail: tsukazaki@tohoku.ac.jp
http://mu.imr.tohoku.ac.jp/index_en.html

Special Symposium : The 50th Anniversary of Superfluid Helium 3 (Hall 1)

Aug. 19 (Fri) (Hall 1) Physics of Superfluid Helium 3 - Past, Present, and Future
Sponsored by JGR Tohoku U
chairs: William Halperin, Keiya Shirahama

19A-S-01	The Discovery of Superfluid Helium-3 (video message)	David M. Lee	Remote	9:00-9:20
19A-S-02	What makes superfluid 3-He special?	Anthony J. Leggett	Remote	9:20-9:50
19A-S-03	Superfluid ^{3}He – *Nature's Gift to Physics*	James A. Sauls	Remote	9:50-10:20
19A-S-04	Superfluid ^{3}He: a perspective on future prospects from materials science to fundamental physics	John Saunders	Onsite	10:20-10:50

Fig. 2 Program of the Special Symposium "The 50th Anniversary of Superfluid Helium 3".

Fig. 3 A group photo at the main Hall.

The 17th 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　神崎展　吉澤晋

Hidemi KATO[1], Hiroyasu KANETAKA[2], Nobuhiro TAKAHASHI[2], Osamu SUZUKI[2], Yoshifumi SAIJO[3], Makoto KANZAKI[3], Shin YOSHIZAWA[3]

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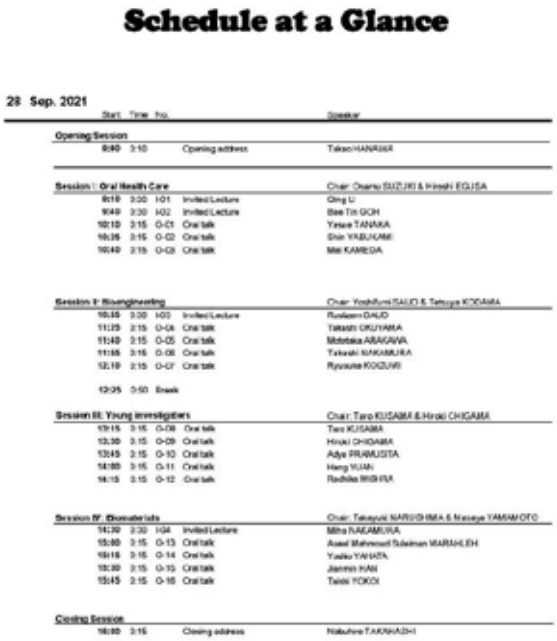
1. 概要

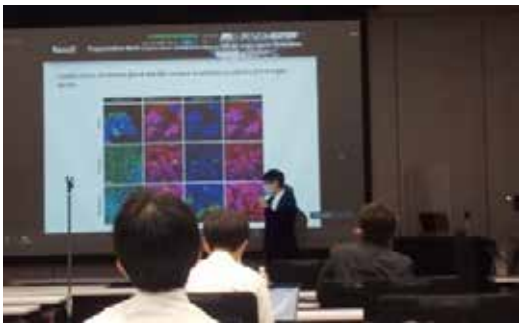
本ワークショップは、生体材料研究を中心とし、材料分野、歯学分野、医工学分野における研究を発表する場を提供する目的で企画されている。主に、東北大学金属材料研究所、歯学研究科、医工学研究科と 3 つの組織で構成されており、それぞれの分野の枠を超えて研究成果を報告することで、研究意義や妥当性を議論できる国際的なワークショップである。また、若手研究者に積極的に参加してもらうことで若手研究者の育成にも繋がっている。

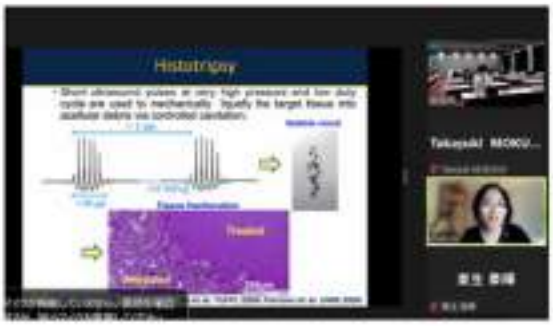
今年度は、オンラインとオンサイトを併用したハイブリット形式で開催され、アメリカ、韓国からも参加があった。内容としては、研究テーマごとに 4 セッションに分けられ、それぞれの研究テーマにおいて、招待講演、口頭発表が行われた。



2. 内容

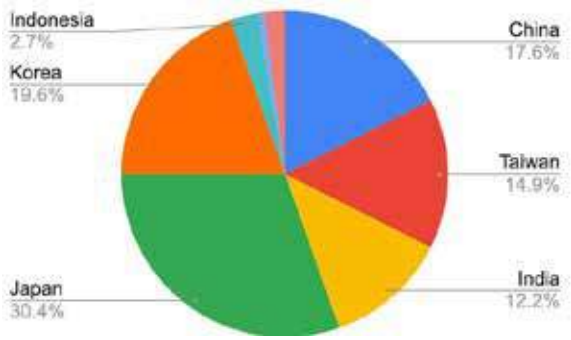
本研究会は、東北大学金属材料研究所、歯学研究科、医工学研究科が連携し、生物-非生物間の現象解明を通してインプラントや人工骨などの生体材料研究の発展を目的とし開催してきた。今年度は、東北大学金属材料研究所講堂を会場とし、オンラインとオンサイトを併用したハイブリット形式で開催した。セッションテーマは、① Oral Health Care、②Biomaterials、③Bioengineering、④ Young innovators の 4 テーマとなり、招待講演者 4 名、口頭発表 16 名であった。招待講演者 4 名のうち韓国ソウル大学の Sangwoo LEE 助教は来日し“Developmental Roles of Hyaluronate and its Biomimetic Application in In vitro Generation of Embryonic Salivary Gland Organ Germ”という題目で発表した。米国ミシガン大学の Zhen XU 教授は、“Noninvasive Mechanical Ultrasound Therapy (Histotripsy) for Cancer Treatment - Latest Progress on Preclinical and Clinical Studies”という題目で、 韓国材料科学研究所の Hui-suk YUN 教授は、“Multi-material 3D Printing Technologies for Bio-applications”という題目で、東京医科歯科大学の梶 弘和教授は、“Drug and Cell Delivery Systems Targeting the Posterior Segment of the Eye”という題目でそれぞれ講演が行われた。オンラインでの参加者が多数ではあったが、最先端の生体材料研究を学ぶことができ、若手研究者、学生、共に研究成果を発表する貴重な場となった。



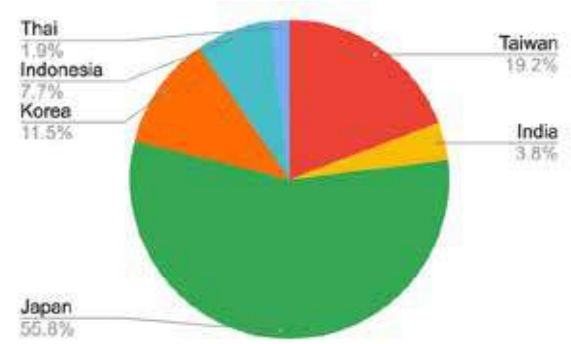


Meeting/conference reports

The Asia-Pacific Conference on Condensed Matter Physics 2022 was held from 21st Nov. to 23rd. Nov. 2022 in Sendai, Japan in hybrid format. This is the 2nd annual meeting of the DCMP. This year, we had APPC15 in summer and so the meeting was focused on three main topics, applications of extreme conditions for condensed matter physics, quantum beam applications in condensed matter physics, topology related phenomena in matters.
The total number of registered participants was 148 and that of the onsite attendants was 52. The 56% of the onsite attendants were from Japan and 19 % were from Taiwan. There were 8 % of attendants from Indonesia.

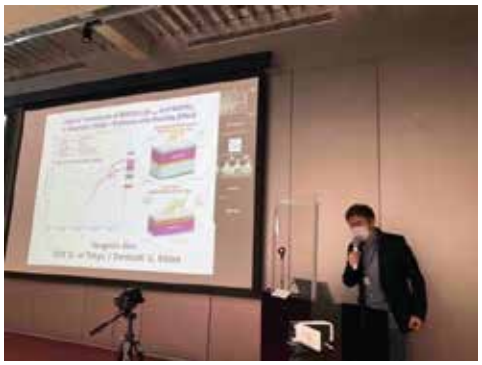


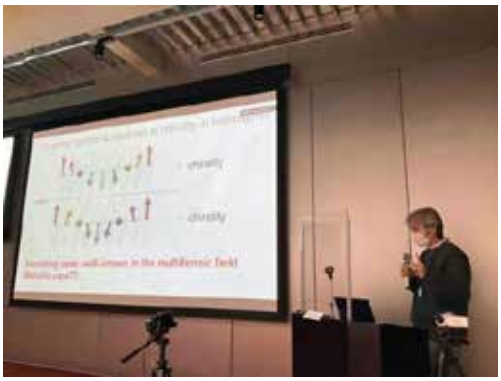
[Composition of registered participants]



[Composition of onsite participants]

The conference started in the morning of 21st with the opening address of the DCMP chair Prof. Park followed by the welcome address from Tohoku University and greeting from Prof. Tajima, the president of the Physical Society of Japan. It was very



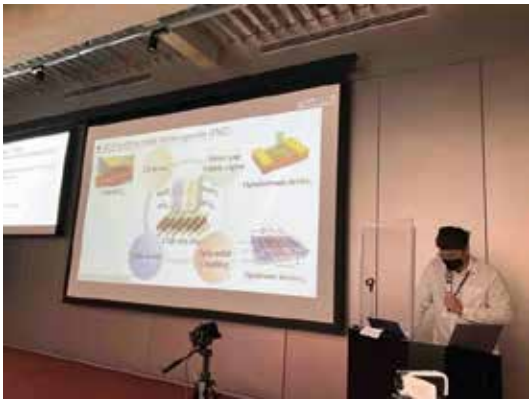


memorable to have two presidents of the physical associations, from Japan and from Taiwan, which are responsible for the current and the future AC2MP meetings.

	Invited	Contributed	Poster
China	6	4	0
Taiwan	6	4	0
India	3	0	0
Japan	4	14	10
Korea	7	3	1
Indonesia	0	2	3
Thai	0	1	0
Others	0	1	0
	26	29	14

Day 1 Program and General Assembly
There were three sessions, Advances in Magnetic and Dielectric Systems, Optical Response and Exotic Magnetic States, Novel Functionality in Matters were hold in the 1st

day with 7 invited, 11 contributed speakers. The keywords of talks are quantum phase



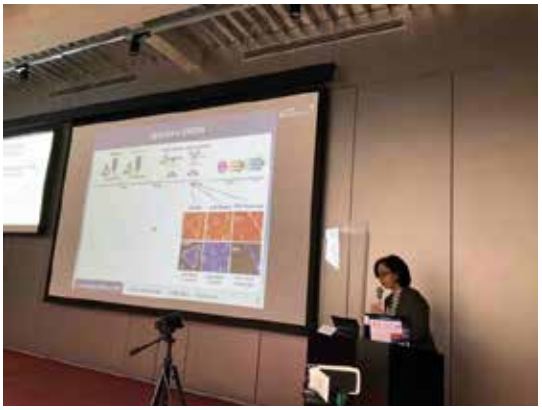
transition, topology, frustration, non-collinear structure, non-linear response, half-metal and others. The talks covered wide

range of the current topics of condensed matter physics with several common key concepts.

In the evening, the General Assembly of the DCMP was hold. The activity report and the election result of the next chair and vice chairs are approved. Prof. Kao and Prof. Ma made the presentation for AC2MP2023 proposal in Hualien, Taiwan from November 27 to 29. and the certificate was given from the DCMP chair to Prof. Kao.

Day 2 Program and Poster Session

There were two sessions about Superconductivity, CDW and Nanoprobes and Physics of Thin Films and Layered Materials. Then poster session with short presentation was held. In the superconductivity session, the discussion on high-T_c superconductivity and the novel superconductive materials were made. In the film and layered materials session, the up to date reports on topological matters and semiconductors were given. The poster presentations from young researchers and students showed the power of the new generations.



Day 3 Program and Poster Session

There were three sessions on Topological Matters and Surface, Nano Science and Novel Transport, Quantum Matters and Extreme Conditions. There were intense discussion on the topology and the transport as well as novel states induced by the strong magnetic fields.The relation between topological matter and strong correlation was also the one of the highlights.

Closing

In the closing remark, the conference chair Prof. Nojiri expressed deep gratitude for attendants, program committee members, the local organizing committee and sponsors for their support and contributions. It was concluded that the meeting was quite successful as the 1st onsite event of the DCMP towards the post covid-19 era.

Budget (tentative)

Travel		
	IMR	APCTP
Invited(Onsite)	549,013	772,602
Speaker(Onsite)	1,166,060	183,740
Others(Onsitw, TBD)		
Invited(Online)		0
Others(Onsite)		
Total	1,715,073	956,342
Others	100,000	

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　佐々木孝彦[1]
研究分担者：東北大材料科学世界トップレベル研究拠点 / AIMR　貞許礼子[2]
Takahiko Sasaki[1], Reiko Sadamoto[2]
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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 on October 24 – 27, 2022.

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、スピントロニクス世界トップレベル研究拠点および大学院プログラム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、2022 年 10 月 24−27 日に第 6 回目となる国際シンポジウムをオンラインにて開催した。なお、今回は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 6 回目となる本国際シンポジウムでは、材料拠点に新しく設置された 4 領域の企画セッションのほか、

スピントロニクス世界トップレベル研究拠点によるセッション、第 5 回目となる材料科学国際共同大学院に参画する大学院生によるセッションの企画運営が行われた。今回はポストコロナやウイズコロナを見据えて、オンラインのみではなく一部ハイブリッドで開催した。4 日間の会期中に海外からの 4 件のプレナリー講演のほか、国内外および学内からの招待講演により材料科学世界トップレベル研究拠点では 4 セッション 12 名、スピントロニクス世界トップレベル研究拠点では 2 セッション 9 名、GP-MS では 5 セッション 20 名の合計 11 セッション 41 名の口頭発表が行われた。また、今回新しい試みとして、シンポジウム会期中 3 日目に東北大学材料科学世界トップレベル研究拠点賞 2022 受賞講演・授賞式を開催し、受賞した 3 名の若手研究者の研究を世界へ発信する機会とした(https://www.crc-ms.tohoku.ac.jp/jp/news/2022/11/02_01_index.html)。シンポジウムのポスターセッションでは、オンラインで 71 件の発表があり、審査により 8 件のベストポスター賞が選ばれ、3 日目に授賞式が行われた。

・参加者：合計 269 名（日本：240 名、海外：29 名）

【セッション概要】

(1)Plenary セッション

・Plenary 講演：4 セッション－海外 4 名

(2)Invited セッション

・材料科学世界トップレベル研究拠点：4 セッション 12 名－学外 12 名(うち海外 5 名)

・スピントロニクス世界トップレベル研究拠点：2 セッション 9 名－学内 3 名、学外 6 名(うち海外 4 名)

・GP-MS：5 セッション 20 名－学内 5 名、学外 15 名(うち海外 14 名)

(3)Poster セッション

・71 件

● 1 日目（2022 年 10 月 24 日）

小谷元子理事・材料科学世界トップレベル研究拠点長の司会による大野英男東北大学総長の開会挨拶に引き続き、折茂慎一材料科学世界トップレベル研究拠点副拠点長を座長として National Tsing Hua University の Prof. Jien-Wei Yeh による“High-entropy materials technology”、Goethe University Frankfurt の Prof. Roser Valenti による“Strategies to design quantum materials with exotic properties”、 ETH Zürich の Prof. Manfred Fiebig による “Seeing is believing: Nonlinear optics on ferroic materials”の 3 件のプレナリー講演が行われた。これに続きポスターセッション 1 が行われた。

● 2 日目（2022 年 10 月 25 日）

午前には、材料科学世界トップレベル研究拠点の“Catalytic and battery materials for carbon neutrality”、 “Cutting-edge measurements of biomaterials and soft matter”の各セッション、GP-MS の学生セッション 1 件が行われた。午後はポスターセッション 2 の後、スピントロニクス世界トップレベル研究拠点から、プレナリー講演として Forschungszentrum Jülich の Prof. Thomas Schäpers による“Topological-insulator-superconductor networks”が行われた後、“Recent progress of magnetic tunnel junction and its application”のセッション、GP-MS の学生セッション 1 件が開催された。

ポスター発表では、オンラインポスターセッションツールを活用した発表およびポスター賞の採点集計が行われた。

・ポスター発表数：71 件－材料科学世界トップレベル研究拠点 23 件、スピントロニクス世界トップレベル研究拠点 35 件、GP-MS 13 件

・ポスター発表表彰：Best Poster Award 8 件

● 3 日目（2022 年 10 月 26 日）

3 日目は材料科学世界トップレベル研究拠点の” Exotic superconductivity”、” Novel high entropy alloys”の各セッション、GP-MS の学生セッション 1 件のほか、材料科学世界トップレベル研究拠点賞受賞講演と授賞式、国際シンポジウムポスター賞の発表と授賞式が行われた。

- 4 日目（2022 年 10 月 27 日）

最終日は、GP-MS の学生セッション 2 件が行われ、及川勝成 GP-MS プログラム長による closing remarks により終了した。

3. まとめ

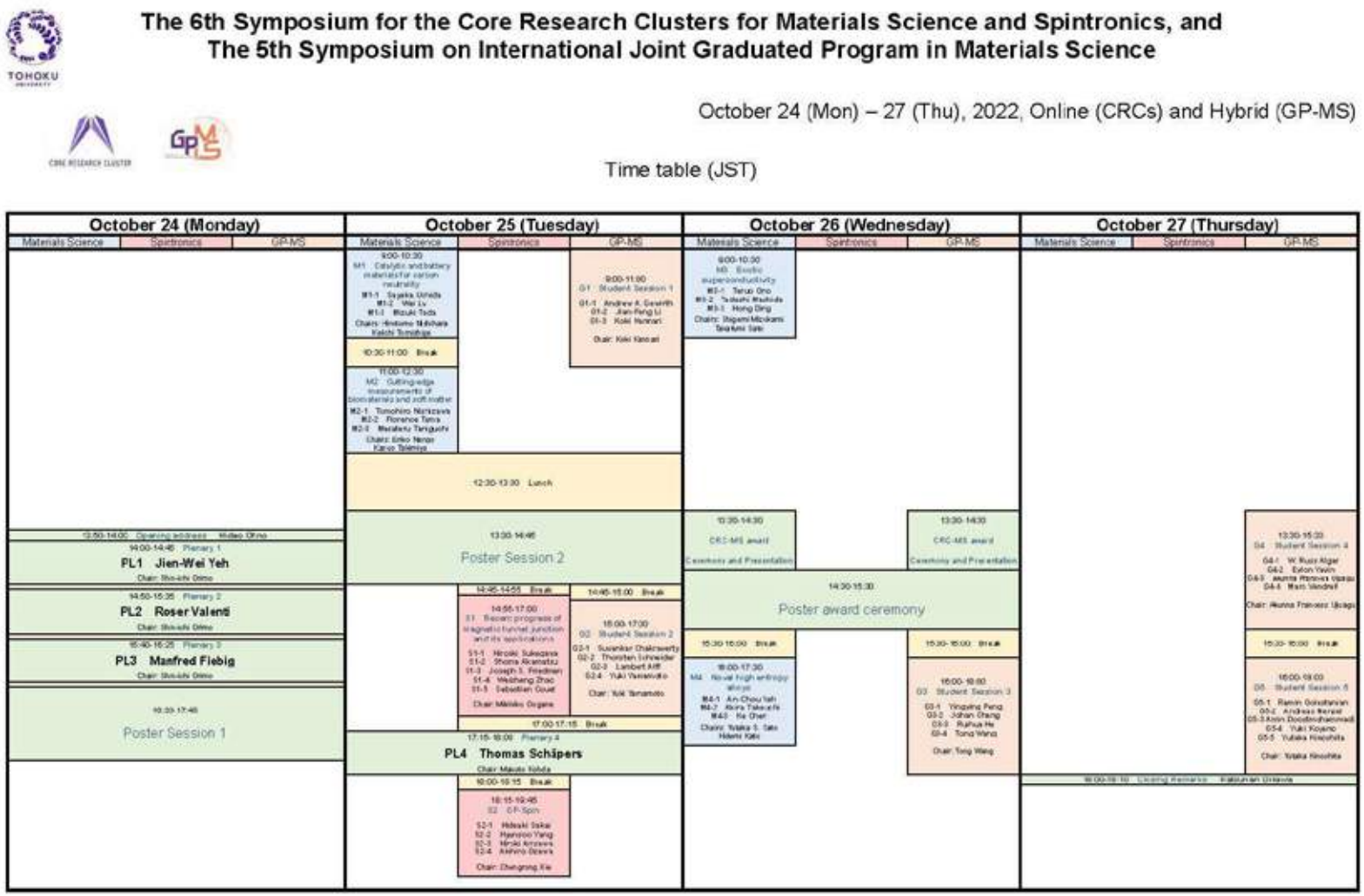
第 6 回となる本シンポジウムは、ハイブリッド開催となり、本学の材料科学分野に関係する多くの部局・拠点・プログラム等の参画により本学の有する卓越したリソースが結集して創出された研究成果を日本の国内外に広くアピールする場となった。次回以降の開催形式は、ポスター発表など特に対面形式を望む声もあることから、今回よりも会場発表を重視しつつ、ハイブリッドの良さを取り入れたものとなるよう計画中である。

謝辞（Acknowledgement）

本シンポジウムは、材料科学世界トップレベル研究拠点、スピントロニクス世界トップレベル研究拠点、材料科学国際共同大学院プログラム(GP-MS)、が主催し、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。運営・企画に参画されたすべての方に謝意を表します。

参考

1) 本シンポジウムホームページ
https://confit.atlas.jp/guide/event/crcgpms2022/top?lang=en2) 本シンポジウムの開催報告ページ
https://www.crc-ms.tohoku.ac.jp/jp/news/2022/11/07_01_index.html
3) シンポジウムプログラム



The 6th Symposium for the Core Research Clusters for Materials Science and Spintronics, and the 5th Symposium on International Joint Graduate Programs in Materials Science and Spintronics プログラム

Activity Report

Young Researcher Fellowships

Young Research Fellowships

No.	Title	Applicant	Affiliation	Host Professor	Proposed Research	Term
22FS01	Ph.D. Student	Thomas Kohne	KTH Royal Institute of Technology,Sweden	Assoc. Prof. Miyamoto	A Study of the Effect of Quenching Rate on the Retained Austenite Stability Using In-situ Tensile Testing in High Carbon Martensitic Steel	2022.7.1-9.20
22FS02	Ph.D. Student	Gionvani Gonccalves Ribamar	University of São Paulo,Brazil	Prof. Furuhra/ Assoc. Prof. Miyamoto	Microstructural Characterization in Quenched and Tempered High Silicon Bearing Steel	2022.7.16-9.16

Impact of cooling rate during martensitic transformation on autotempering

The relation of cooling rate, martensite tetragonality and autotempering behavior was studied for two cooling rates. The slower cooling rate showed epsilon carbide precipitation, while no carbides were observed for the faster cooled sample even after short tempering. Additionally, a new approach for local martensite tetragonality determination was introduced.

Previous work by Kohne et al. [1,2] showed the significant impact of cooling rate during the martensitic transformation on the martensite tetragonality and carbon distribution and a heterogeneous distribution of both was observed. Atom probe tomography showed carbon clustering, but the results regarding carbide formation during cooling were not conclusive [2]. Therefore, the effect of cooling rate and local tetragonality on the autotempering kinetics in a high carbon steel was investigated during the visit at Furuhara Laboratory.

Three heat treatment conditions, 'fast', 'slow' and 'fast + tempered', were carried out and consisted of austenitization of the samples followed by cooling to room temperature with a change in cooling rate at 260 °C. The 'fast' sample had a cooling rate of approximately 30 °C/s to room temperature and the 'slow' 0.5 °C/s. The 'fast + tempered' condition is the sample 'fast' with an additional 3 min tempering at 180 °C.

In the next step, the local tetragonality was determined by electron backscatter diffraction (EBSD). In previous work [1,2], the method of Winkelmann et al. [3] has been used, but it was not possible due to the low fraction of austenite.

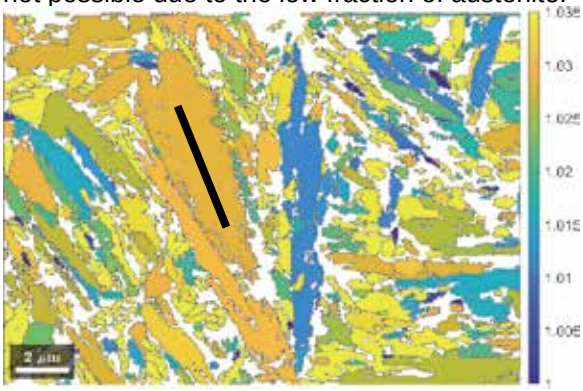


Fig. 1 Local martensite tetragonality for 'fast'

Therefore, an approach for determination of average tetragonality of EBSD maps that was developed in Furuhara Laboratory was used. It was extended to local determination of tetragonality by averaging over all pixels of each martensite unit. The resulting tetragonality is shown in Fig. 1 for the fast cooled sample. The heterogeneous distribution of martensite tetragonality is clearly visible. Transmission electron microscope (TEM) specimens were prepared by focused ion beam (FIB) lift-out based on the local tetragonality. The black line in Fig. 1 indicates the position of the FIB lift-out. For 'slow', a region of low tetragonality was chosen and for 'fast' a region of high tetragonality. The 'fast + tempered' specimen was taken from an area that had high tetragonality before tempering determined by previous EBSD scans.

In TEM, the specimens were investigated with bright and dark field (DF) as well as high resolution TEM and diffraction. The DF imaging showed elongated precipitates for sample 'slow', see Fig. 2. These precipitates were determined to be eta carbides by TEM diffraction. The 'fast' and 'fast + tempered' samples showed no conclusive evidence of carbides in DF and diffraction.

Overall, a new method for the local determination of martensite tetragonality was developed and further validation and comparison with existing methods is ongoing. Additionally, the clear difference in autotempering behavior for different cooling rates during the martensite transformation was shown.

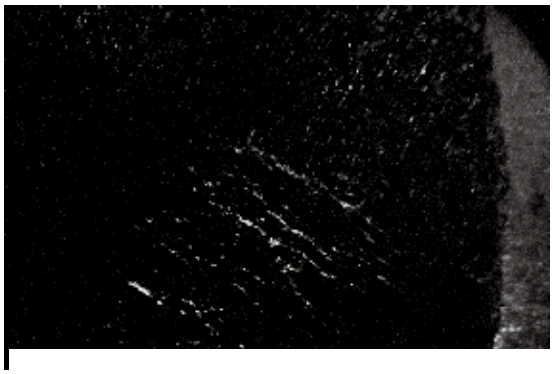


Fig. 2 DF TEM image of eta carbides of 'slow'

References

[1] T. Kohne, et al. Metall Mater Trans A 54(4) (2023).
[2] T. Kohne, A. Dahlström, A. Winkelmann, P. Hedström, A. Borgenstam, Materials, 15(19) (2022)
[3] A. Winkelmann, G. Nolze, G. Cios, T. Tokarski, Phys. Rev. Mater. 2(12) (2018)

Keywords: Martensite, Martensite tetragonality
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Microstructural Characterization in Quenched and Tempered High Silicon Bearing Steel

Silicon alloying holds promise for chemical and mechanically stabilizing retained austenite in steels by enriching carbon. However, limited investigations have been conducted on high-carbon bearing steels, which could enhance toughness without compromising wear behavior. This study presents our results, emphasizing microstructural characterization of a high-carbon, high-silicon bearing steel.

High-carbon bearing steels possess excellent hardness, wear resistance, and dimensional stability. However, their limited toughness and ductility impose limitations and shorten the lifespan of components. Although retained austenite, commonly found in commercial steels, can improve those properties, it can also transform into brittle fresh martensite with high carbon content during use, resulting in dimensional changes due to the natural expansion of martensitic transformation.

Nevertheless, alloying with silicon has been proven effective in stabilizing austenite by increasing carbon enrichment to levels that prevent its transformation into martensite [1]. Microstructural analysis of the studied alloy revealed no significant changes up to 200 °C, while atom probe tomography found carbon redistribution within the martensite, likely due to dislocations. Transmission electron microscopy revealed the formation of η-carbide after tempering at 250 °C.

Fig. 1a and 1b depict the quantification of austenite phase and carbon content evolution during continuous heating tempering. Austenite volume fraction showed a slight decrease at two temperature ranges termed “A” and “B”, attributed to the limited formation of ferritic bainite (Fig. 1d), observed after quenching from 400 °C. The bainite morphology displays small leaf-like structures cutting through the retained austenite. No significant decomposition of austenite is noted within the “C” temperature range. However, the retained austenite in this range exhibits a high carbon content, indicating mechanical stabilization with a stacking fault energy exceeding 30 mJ.m^{-2}, making transformation unlikely under applied strain. At 530 °C, austenite gradually loses carbon and decomposes into cementite particles (θ_S), distinct from spheroidized cementite formed during intercritical solubilization, as confirmed by TEM analysis. Within the “D” temperature range, austenite rapidly loses carbon and decomposes into ferrite and cementite.

The results demonstrate a temperature range where austenite can be rapidly thermally and mechanically stabilized, avoiding significant decomposition or the formation of undesired cementite. Silicon alloying showed to be highly effective, even in high-carbon steels, in delaying cementite formation and facilitating austenite stabilization. Austenite stabilization achieved within the 400-470 °C temperature range is sufficient to prevent transformation-induced plasticity effects in bearing steels, improving toughness and ductility while maintaining its good dimensional stability.

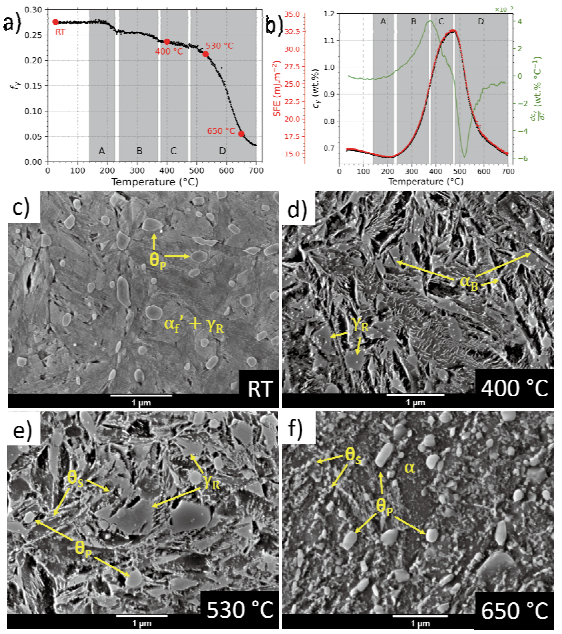

Fig.1 – a) austenite volume fraction and (b) austenite carbon content evolution during tempering at continuous heating. SEM micrographs of (c) initial microstructure and after immediately quenching from: (d) 400 °C, (e) 530 °C, and (f) 650 °C.

References

[1] G.G. Ribamar, J.D. Escobar, A. Kwiatkowski da Silva, N. Schell, J.A. Ávila, A.S. Nishikawa, J.P. Oliveira, H. Goldenstein, Acta Mater. 247, 118742 (2023).

Keywords: Alloy, Steel, Phase Transformation
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Activity Report

IMR Young Fellowships for Graduate Students

IMR Young Fellowships for Graduate Students

No.	Title	Applicant	Host Professor	Proposed Research
22YFP01	Ph.D. Student	Liu Weiqi	Prof. Ichitsubo	Research on the Development of Electrode Materials in Rechargeable Batteries
22YFP02	Ph.D. Student	Zheng Bohao	Prof. Furuhara	Control of Grain Boundary Segregation in Ferrite Using Interaction Between Solute Elements
22YFP03	Ph.D. Student	Tao Zhang	Prof. Chiba	FEM Analysis for Laser DED Process
22YFP04	Ph.D. Student	Yunhe Zhou	Prof. Chiba	A Study on the Development of Superalloys Such as Co Alloys by Electron Beam Lamination (EBM) Technology
22YFP05	Ph.D. Student	Zheng Jiajie	Prof. Fujita	Sample Preparation of T*-type Cuprate for μSR Measurements
22YFP06	Ph.D. Student	Weida Yin	Assoc. Prof. Seki	Study of Anomalous Nernst Effect in Ferromagnetic Ternary Nitride Films
22YFP07	Ph.D. Student	Theo Sasha Balland	Assoc. Prof. Seki	Spin Injection Into a Nonmagnetic Semiconductor by Spin-Pumping
22YFP08	Ph.D. Student	Tan Yuan	Prof. Ichitsubo	Improving the Cycle Life of Storage Battery Materials Through Structural Control
22YFP09	Ph.D. Student	Jeong Jiyeong	Prof. Furuhara	Effects of Mn on Liquid Metal Embrittlement of Zn-coated Steels
22YFP10	Ph.D. Student	Ji Ke	Prof. Miyasaka	Development of Conductive Organic Polymers Carrying Carboxylate-Bridged Paddlewheel Diruthenium(II,II) Units
22YFP11	Ph.D. Student	Louis Lesage	Prof. Kato	Processing of Micro-Porous Metallic Powders by Liquid Metal Dealloying

Development of Aluminum-foil Anode for Lithium Batteries

Abstract: Aluminum foil has a very high theoretical capacity and can be used as an anode material with an active material and a collector, which is a promising feature of anode materials for rechargeable lithium batteries. However, the aluminum foil disintegrates due to volume shrinkage during the charge/discharge cycle. In this study, we prepared different aluminum foil alloys and explored the effect of added alloying element zinc on the aluminum foil.

For lithium-ion batteries, alloy-based anode materials have higher theoretical capacity than conventional carbonaceous anodes, but the large volume change accompanying the lithiation and delithiation causes significant structural degradation. We have developed the first as-rolled Al foil (99.99%) anode that serves as both active material and current collector[1]. However, as the as-rolled Al foil anode, when the lithiation process occurs, the Al matrix regenerated on the electrode surface has a lower intragranular diffusion rate of Li compared to LiAl. As a result, Li diffusion from the grain boundaries is more likely to progress, and the Al matrix becomes excessively porous as a result of grain boundary breakdown (the self-organization of Al foil).

In this work, we used sputtering method to coat the as-rolled Al foil with a layer of zinc. Two-electrode coin-cells were used for electrochemical measurements to study the lithiation behavior. Ternary oxides were used as cathode materials.The crystal structures of the synthesized samples were characterized by x-ray diffraction.

Fig.1 shows the changes in the crystal structure of the Al and Al-Zn foil anode before and after reaction behavior of Zn. The experimental results showed that Zn coated on the Al foil surface solidly dissolved into the LiAl phase as a result of Li alloying, improving the initial irreversible capacity at the time of Li desorption.

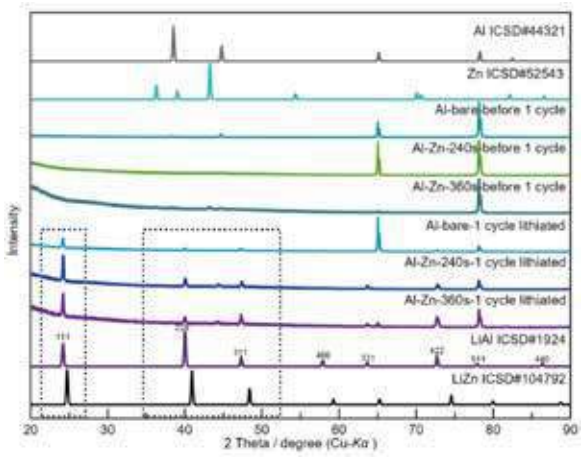

Fig 1. XRD of Al-Zn foil before and after lithiation

Fig. 2 shows the charge-discharge curves of the as-rolled Al foil coated with a layer of Zn. From this result, we can find the improvement of cycle stability is still little. However, the initial irreversible capacity lost during the first cycle is greatly reduced, which is good sign.

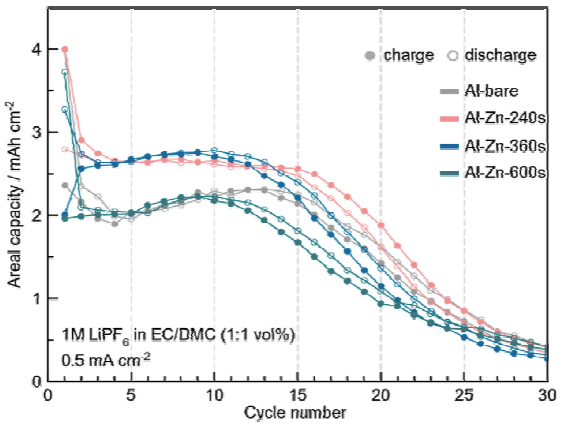

Fig 2. the charge-discharge cycle curves of Al-Zn foil anode

In the future, we will consider different methods of Al(as rolled)-Zn alloying, increase the proportion of Zn in the alloy and explore the effect of Zn on the as-rolled Al foil.

References

[1] Li, H. *et al,* Nat. Commun. 11, 1584 (2020).

Keywords: Electrical Properties, Alloy, XRD
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Controlling Grain Boundary Segregation by Solute-Solute Interactions

Abstract: carbon is known to being able to increase the binding energy of grain boundaries (GBs) in bcc Fe and suppress the harmful segregation of phosphorus along GBs. This research aims to understand the interactions between different solutes around GBs and to utilize such interactions to further suppress the segregation of phosphorus at GB sites. This article reports the outline our research, as well as some of the early progress.

Phosphorus is known to cause tempering embrittlement of steels by segregating at grain boundaries, which reduce the binding energy of grain boundaries (GBs). Modern steelmaking practices can reduce phosphorus content to ~100 ppm [1]. But in order to obtain steels with higher strength and toughness, it is necessary to understand the segregation behavior of phosphorus at grain boundaries and thus develop suppression procedures. Our past research [1,2] have confirmed that carbon acts as a suppressor for P segregation. Based on this previous knowledge, our current research aims to further investigate the segregation behavior of carbon and its interaction with substitutional solutes in bcc iron utilizing both experiment and simulation approaches.

For the experiments, we plan to investigate the GB segregation behavior of binary Fe-1Si and Fe-1Mn samples as well as their carburized counterparts. Based on our previous findings [1,2], when investigating the segregation, we also take the influence of GB character (i.e., tilt and twist component of the GB) into account. In order to fully determine the five macroscopic degrees of freedom (DOFs), electron backscatter diffraction (EBSD) and focused ion beam (FIB) are used. Fig. 1 shows the schematic diagram of FIB observation, and the example results of this process.

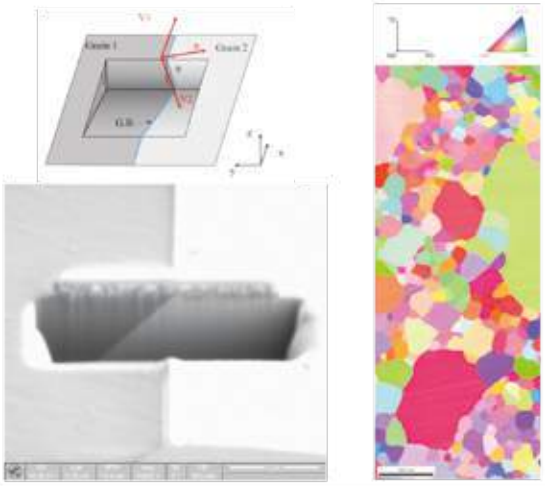

Fig. 1 (Clockwise from right) EBSD orientation map of the sample; actual and schematic FIB image of the GB trace.

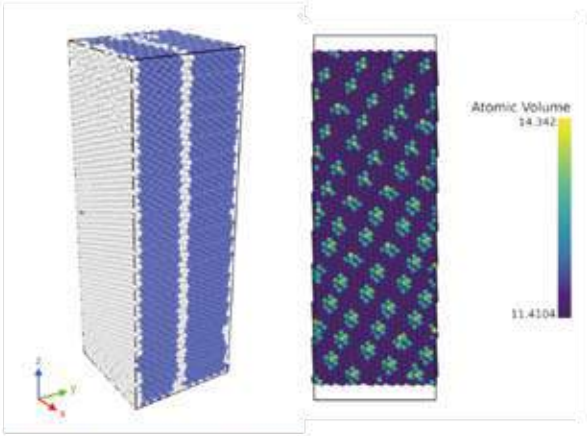

Fig. 2 Typical atomic model for the simulation (left) and the cross section along GB plane showing atomic volume by Voronoi analysis

For the simulation part, we're currently developing a workflow that allow us to identify all the interstitial segregation sites in the atomistic models. With a hybrid molecular statics – Monte Carlo (MS-MC) simulation scheme similar to that by [3], we would be able to gain insight on the spectra of stie-specific segregation energy and the interactions between solute elements. Furthermore, the influence of segregation entropy can be incorporated into the simulation by molecular dynamics. Fig. 2 shows the atomistic model of bcc iron with specific GBs.

References

[1] K. Ikeda, Tohoku Univ. Master Thesis (2020).
[2] K. Yamasaki, Tohoku Univ. Master Thesis (2021).

Keywords: steel, grain boundaries, simulation
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Microstructure control of interface layer between Fe based- and Al based-alloys by using directed energy deposition (DED) type additive manufacturing

In recent years, directed energy deposition (DED) type additive manufacturing has been applied in many industries. To meet the demand for high strength and rigidity of metal parts with lightweight, Fe/Al multi-material system is of increasing importance. The significant differences in physical properties of Fe and Al, and the formation of intermetallic phases will directly deteriorate its mechanical performance. Therefore, this research is aimed to optimize the DED processing parameters to improve the microstructure and mechanical properties.

In this study, spherical Al3SiMn powders were used. Additional powder sieving was applied to achieve the best print results. The surface morphology of the Al3SiMn alloy powder was observed using a scanning electron microscope. As received SS 304 plate with a thickness of 10 mm was selected as a metal substrate. The samples were fabricated by LAMDA 200 DED device (Mitsubishi Heavy Industries, Ltd., Japan).

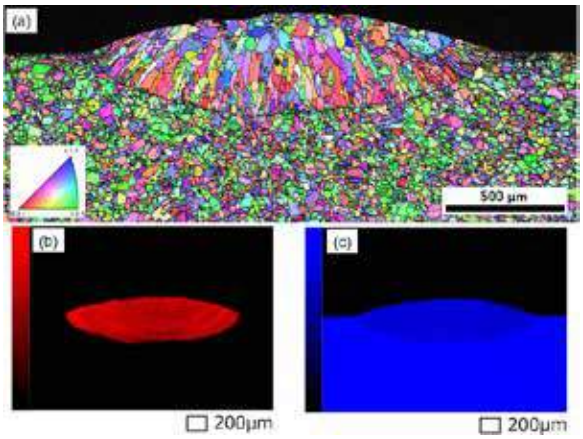

Fig 1. EBSD and EDS results of sample fabricated with low powder feeding rate. (a) IPF Map. (b) Al distribution. (c) Fe distribution.

Fig.1(a) shows IPF map of sample processed with laser power of 800W and low powder feeding rate of 1.6 g/min. The EBSD result suggests that the microstructure of heated affected zone and substrate is mainly composed of equiaxed crystals. While the fusion zone has columnar crystal microstructure, which has the morphology of epitaxial growth along the fusion zone. Besides, no intermetallic compound occurs in the process parameter of low powder feeding rate.

The EDS elemental distribution analysis was performed at the cross-section of sample which processed at low powders feeding rate. From Fig 1(b) and (c), we can find that Al uniformly distributed at the fusion zone whereas Fe distributed at both fusion zone and substrate zone. Furthermore, the concentration of Fe is higher at substrate than fusion zone. Combining with IPF map, we can infer that, solid solution might be formed by the solution of Al atoms into Fe lattice in molten pool.[1]

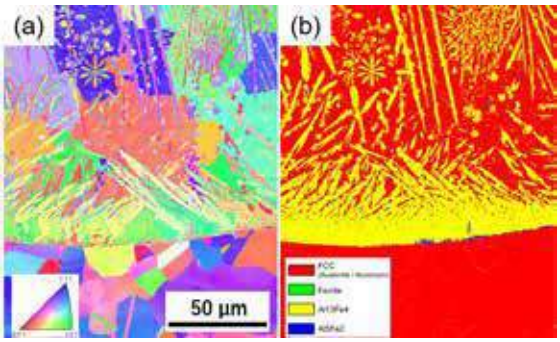

Fig 2. EBSD results of sample fabricated with high powder feeding rate. (a) IPF Map. (b) Phase distribution.

Another sample was prepared with the same power of 800W but higher powder feeding rate of 6.4 g/min. The IPF map at the cross-section of this sample was demonstrated in Fig 2(a). The intermetallic layer was formed at the interface of Fe and Aluminum. Columnar dendrites in the fusion zone turn out to be $Al_{13}Fe_4$ intermetallic compound.

In conclusion, the intermetallic compound is more likely to form with the increasing of the powder feeding rate.

References

[1] A. Emdadi, S. Bolz, J. Buhl, S. Weiß, and M. Bambach, Metals. 12, 997. (2022).

Keywords: Microstructure, Steel, Dendrite
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Microstructure, electroconductivity, and mechanical performance of Cu-5 wt.% Ag alloy fabricated by electron beam powder bed fusion

Abstract : Cu-Ag alloys have excellent comprehensive properties such as electrical conductivity, thermal conductivity, and mechanical mechanics. As conductors and key structural components, they are widely used in many fields such as electronic information, electricity, energy, machinery, aerospace [1]. In this study, an additively manufactured sample of Cu-5Ag alloy was successfully fabricated by electron beam powder bed melting technique. The effect of processing parameters on the microstructure and electrical conductivity and tensile properties of the alloy was explored.

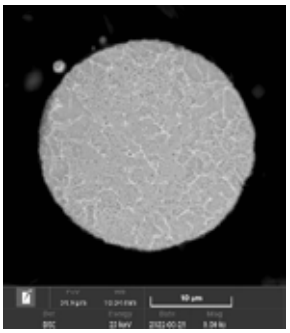

Fig.1 shows the transverse area of Cu-5Ag powder. EDS results exposed that the white curves are the precipitates of Ag along the grain boundary.

Fig.2 shows the additive manufactured sample in electron beam powder bed fusion machine.

Powder characteriazation:

Content: 95 wt.%Cu+ 5 wt.% Ag

Manufacturing method: Gas atomization.

Experiments:

- Density test
- SEM-BSE
- TEM
- EBSD
- XRD
- Optical Microscopy
- Electrical conductivity test
- Tensile test
- Hardness test
- Flow 3D simulation

Manufacturing parameter:

- Dimension: 30x30x11 mm
- Current: 24,27,30mA.
- Scanning speed: 2000, 2400, 2800mm/s
- Lineoffset: 0.1 mm.

Introduction:

Applying different combination of the selected current and scanning speed, the linear energy density of the electron beam is changed in a gradient manner to obtain nine additively manufactured copper alloy samples with different microstructures and mechanical properties. No. 3, No. 6, and No. 9 samples showed obvious edge warping. The other five samples except these 4 samples all present better appearance and compactness. When the electron microscope observation and backscattered electron diffraction test were carried out on the nine samples, it was found that the microstructure, the mechanical properties and electrical conductivity showed regular differences with the printing parameters. The study found that due to the severe non-equilibrium solidification caused by the ultra-high cooling rate, the additive manufacturing samples presented different microstructures from those of traditional casting and powder metallurgy copper alloys. Fine columnar and equiaxed crystals are found. The sample has property anisotropy and showed better mechanical and electrical properties along the additive direction compared with the Cu-Ag alloys under the traditional manufacturing method.

References

[1] Gong, X. (2021). Microstructure and property evolution mechanism of Cu-5wt.%Ag alloy regulated by Ag precipitation (PhD thesis).

Keywords: Electrical Properties, Alloy, Mechanical Prorerties
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Research on the second phase of T'-type cuprate superconductor containing Praseodymium, Lanthanum, Nickel and Cerium

Abstract: It was found by X-ray diffraction that the cupric acid superconductors with praseodymium and lanthanum, which were supposed to be T '- type materials, would have a T-type second phase structure when the amount of lanthanum doping was too large. And after doping nickel, the amount of lanthanum doping required for the emergence of the second phase will be reduced.

In 1986, J.G.Bednorz and K.A.Muller discovered cuprate high-temperature superconductors mainly characterized by high Tc (critical temperature). So far, much of the research on cuprate high-temperature superconductors has been on compounds known as the 214 series. The reason is their simple structure with only two CuO2 surfaces per unit lattice makes it easier to understand what happens inside them. On the other hand, by substituting a small amount of elements for the original substance, the physical properties of the obtained new substance may have obvious changes. Therefore, in order to understand the universal superconducting mechanism, it is necessary to study the similarities and differences between the original material and the electron-doped material through systematic experiments.

To research these substances, is usually used to make them. The raw materials are fully ground and mixed and then heated, dried, and tableted for several times to form polycrystals of the desired substance.

The 214-series cuprate superconductors studied in the laboratory are classified into structural isomers: T-type, T'-type, and T*-type

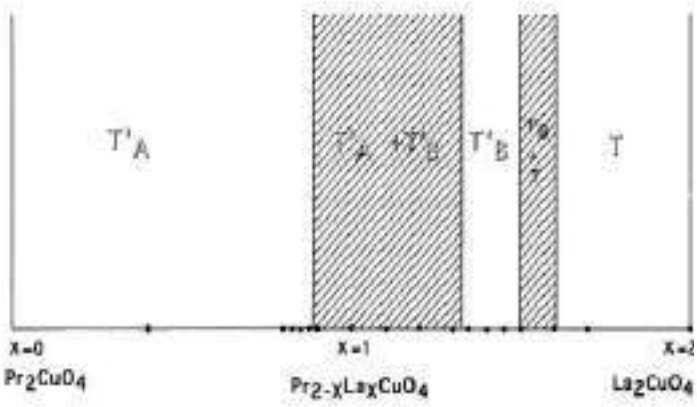

Fig.1 Phase relationship for the tie line between the change of x. [1]

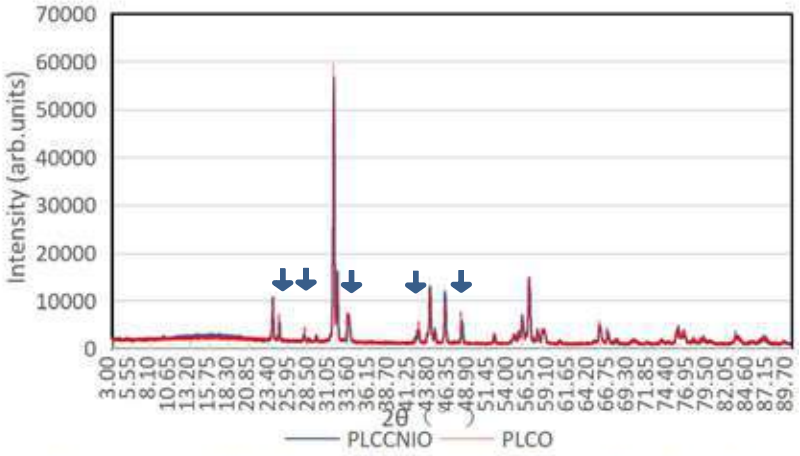

Fig. 2 X-ray diffraction picture of $PrLaCuO_4$ (PLCO) with higher lanthanum content and PLCCNIO (PLCO doped with cerium and nickel).

structural isomers: T-type, T'-type, and T*-type according to the coordination number of oxygen ions around copper ions. The original substance of the T'-type material represents Pr2-xLaxCuO4. Since the T'-type structure is not stable, its content of lanthanum increases, that is, T-type and T' will appear in the case of 1.45<x<1.6 -type coexistence of two phases. (see Fig.1)

Prepared by the method, and a small amount of nickel is added to replace copper, the new substance synthesized is $Pr_{0.92}LaCe_{0.08}Cu_{0.92}Ni_{0.08}O_4$. The structure of the new material was determined by X-ray diffraction. The obtained results are compared with the traditional T 'structure and the diffraction spectra of two-phase coexisting materials. (See Figure 2). It can be seen that even if the lanthanum content x in this material does not exceed 1.45, it still presents an All four characteristic peaks of the T-type structure. Undoubtedly, this type of new substance is a substance in which T-type and T'-type structures coexist in two phases.

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Anomalous Nernst Effect in $Fe_{4-x}M_xN$ (M=Ni, Co, and Mn) Films Grown by Molecular Beam Epitaxy

A thermoelectric power generator can transform waste heat to electric energy without pollution and noise. The anomalous Nernst effect (ANE) is a kind of a thermoelectric effect that can generates an electric field orthogonal to both magnetization and temperature gradient in ferromagnetic materials. The purpose of my research is to study the ANE of $Fe_{4-x}M_xN$ (M=Ni, Co, and Mn) films.

Fe_4N possesses an anti-perovskite lattice structure, in which Fe atoms occupy the corner and face-centered sites and an N atom occupies the body-centered site. Fe_4N is a promising material with relatively large anomalous Nernst coefficient (S_{ANE}) [1]. In addition, substitution of the Fe atoms in Fe_4N with other 3*d* transition metals are an effective method to modify the electrical and magnetic properties of Fe_4N. The fabrications, characterizations, and first-principles calculations on $Fe_{4-x}M_xN$ (M= Ni, Co, and Mn) have been reported in several papers [2-4]. However, there are no reports on S_{ANE} in $Fe_{4-x}M_xN$. Thus, based on the previous research, in my study, $Fe_{4-x}M_xN$ films were fabricated and their S_{ANE} values were characterized to reveal the Ni, Co, and Mn addition effect to Fe_4N.

In order to investigate S_{ANE}, $Fe_{4-x}Ni_xN$, $Fe_{4-x}Co_xN$, and $Fe_{4-x}Mn_xN$ films were fabricated on $MgAl_2O_4(001)$, $(LaAlO_3)_{0.3}$-$(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}(001)$, and MgO(001) substrates, respectively, by molecular beam epitaxy. After the growth of the films, The atomic ratio (x value), thickness, and the structure of the films were characterized by electron probe micro analyzer, x-ray reflection, and x-ray diffraction (XRD), respectively. The saturation magnetizations of the $Fe_{4-x}M_xN$ films were measured by a vibrating sample magnetometer at room temperature. After the characterization of the films, the samples were microfabricated into a Hall bar shape by using Ar ion milling and photolithography for the measurements of transport phenomenon like ANE, the Seebeck effect, and the anomalous Hall effect.

In this report, the results on $Fe_{4-x}Ni_xN$ films are shown. The cube-on-cube epitaxial relationship between the $Fe_{4-x}Ni_xN$ films and the $MgAl_2O_4(001)$ substrates were confirmed from the in-plane and out-of-plane XRD patterns, but the $Fe_{4-x}Ni_xN$ phase started to decompose into FeNi at about x = 2.3. The relationships among S_{ANE}, Seebeck coefficient (S_{SE}), and x in the $Fe_{4-x}Ni_xN$ films are shown in Fig. 1. The S_{ANE} value decreases from 1.7 to 0.6 μV/K and the S_{SE} value increases from -2.3 to 1.2 μV/K with x. By using the experimental data, the transverse thermoelectric conductivity (α_{xy}) was calculated. The result shows that α_{xy} decreased with x and the change of α_{xy} is dominated the change of S_{ANE}.

Thus, in order to enhance the S_{ANE} value of $Fe_{4-x}M_xN$ films, we need to find the element which can improve the α_{xy} of $Fe_{4-x}M_xN$.

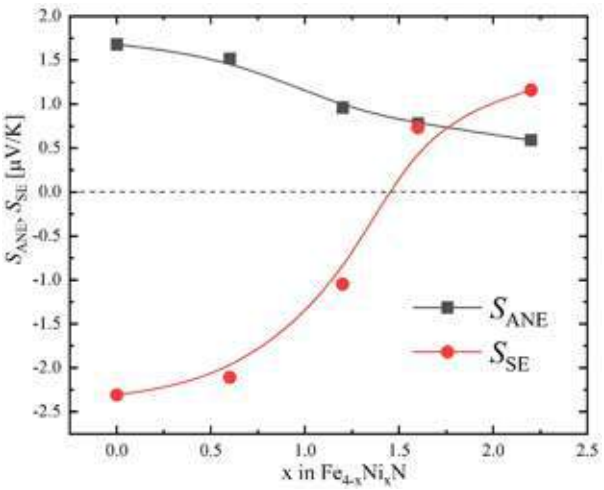

Fig. 1 The S_{ANE} and S_{SE} of $Fe_{4-x}Ni_xN$ films as the function of Ni composition.

Besides the experiments and the life in laboratory, I also participated in several domestic and international conference and made oral presentations. I really enjoy the life in Sendai, Japan, and appreciate that ICC-IMR have supported me to come to Japan to feel Japanese culture, obtain knowledge, and do research.

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Keywords: Spintronics, Thermoelectric, Molecular Beam Epitaxy
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Spin injection based on spin pumping in microfabricated ferromagnetic metal/nonmagnetic semiconductor junctions

Electron spin wave is spatial spin rotation of electrons moving through an effective magnetic field generated by spin orbit interaction in semiconductors. Its integration in semiconductor devices for novel wave-based parallel computing technology requires efficient spin injection, transport and detection. In this study, we investigate the efficient injection of spin current in microfabricated devices by exploiting the spin pumping.

In order to develop wave-based parallel computing using the electron spin wave, this study exploiting spin pumping for spin injection and inverse spin Hall effect (ISHE) for spin detection. The spin pumping injects a spin current into a semiconductor layer thanks to the RF excitation of the magnetization dynamics in an adjacent ferromagnetic layer. The inverse spin Hall effect convert the spin current into a transverse charge current. As a first step to electrically create the electron spin wave, in this study, we have investigated the injection of spin current from a CoFe ferromagnetic layer into a GaAs by conventional non-local spin-valve (NLSV) technique. Based on the knowledge obtained by NLSV experiment, we have designed the microfabricated device working with the spin injection by spin pumping.

First, the devices of NLSV were fabricated. The size of injection electrode is 10 µm x 1 µm while that of the detection electrode is 10 µm x 500 nm, which are separated by a channel of *l* = 500 nm, 700 nm, 900 nm and 1200 nm. Magnetoresistance measurements were conducted and these devices exhibit clear NLSV signal at temperatures lower than 200 K. The amplitude of this signal increases as the temperature decreases. Fig.1 shows the typical measured NLSV signal.

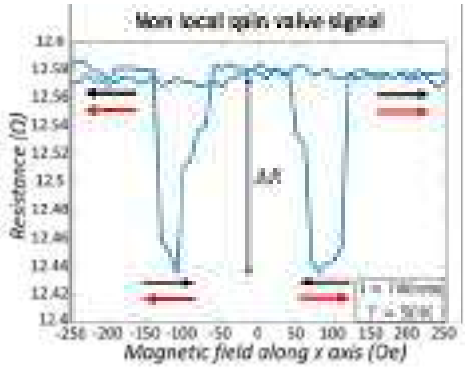

Fig. 1 Non local spin valve signal for CoFe / GaAs device measured at 50 K. The black and red arrows denote the magnetization alignments.

The observation of NLSV signal suggests that the present microfabrication process has successfully been optimized and that a spin signal can be detected in a microfabricated structure with a channel length between 500 and 1200 nm.

Then, we conducted the Ferromagnetic resonance (FMR) measurements with the spin pumping electrode by applying a RF current and a sweeping magnetic field. The preliminary results were conducted on a reference electrode made of Permalloy (20 nm thick) and Pt (4 nm thick). The electrode exhibits a characteristic FMR spectra which means magnetization precession dynamics can be excited in a 10 µm x 1 µm electrode. The FMR signal depends on the applied magnetic field orientation (at 0°, the magnetic field is perpendicular to the electrode). Fig. 2 shows this magnetic field orientation dependence of the FMR signal.

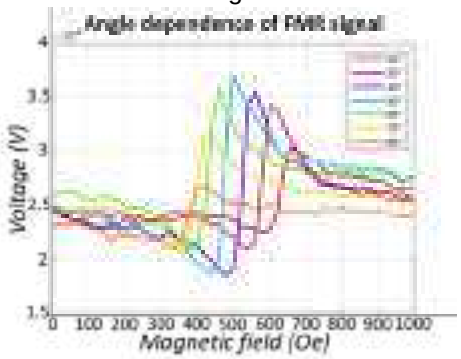

Fig. 2 FMR spectra for the microfabricated device with Permalloy/Pt bilayer.

In the future work, these results and obtained knowledges will be used for the experiment controlling the electron spin wave.

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Research of relationship between structural inhomogeneity and relaxation in metallic glass

Abstract: Metallic glass is eye-catching for its excellent properties and potential utilization. However, as an amorphous material, there remain difficulties, one of which is how the interaction between structural inhomogeneity and relaxation happens in metallic glass. In this research, we will compare kinds of metallic glass in similar glass transformation temperature for discovering correspondence of microstructure and relaxation phenomena.

The microstructure of substance can be divided into two classification, amorphous structure and crystal structure. Metallic glass, as a kind of amorphous substance made from metal atoms, has been a novel field for its young history and potential utilization. Metallic glass, of which the structure is glassy-like, can be classified into fragile to strong one. Viscosity of fragile metallic glass near glass transformation temperature (T_g) changes suddenly while the strong one shows an even tend of change. Research from our lab has revealed a possible forecast that the structural inhomogeneity, consisting of strongly bounded regions (SBR) and weakly bounded regions (WBR), is inside a typical fragile bulk metal glass PNCP ($Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$)[1]. It also be discussed that WBR is more easily to be influenced, where reactions occur. Left picture of Fig.1 shows that observed grey region is the amorphous area inside the metallic glass.

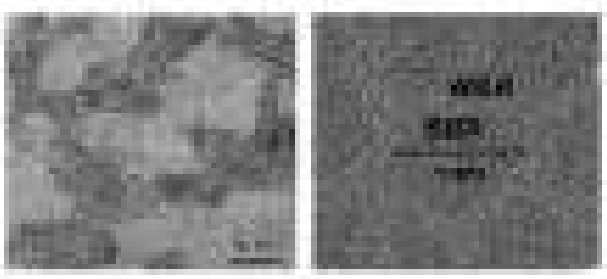

Fig. 1 (Left) HREM image of partially crystallized PNCP; (Right) The Inferred inhomogeneous structure model of metallic glass.

The structural inhomogeneity can also be detected by change of enthalpy happened during process of heating up over crystallization temperature (T_x) via Differential Scanning Calorimetry (DSC). Comparing DSC data of bulk metallic glass (BMG) after quenching and BMG annealed at sub T_g, a heat-absorbing peak before T_g was found, which is called shadow glass transition, and it is revealed to be respect to β structural relaxation during long-time annealing[2]. The thought-provoking point is that what relationship of fragility and shadow glass transition.

Our group will focus on three kinds of metallic glass from fragile to strong, which are called Vit101($Cu_{47}Ti_{34}Zr_{11}Ni_8$), Vit105($Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$), and Vit106($Zr_{57}Cu_{15.4}Ni_{12.6}Al_{10}Nb_5$) with similar glass-transition temperature around 680K. Fig.2 shows that fragile Vit101 has the lowest T_g while strongest Vit106 has the highest T_g. Furthermore, difference from T_g to T_x is increasing from Vit101 to Vit106.

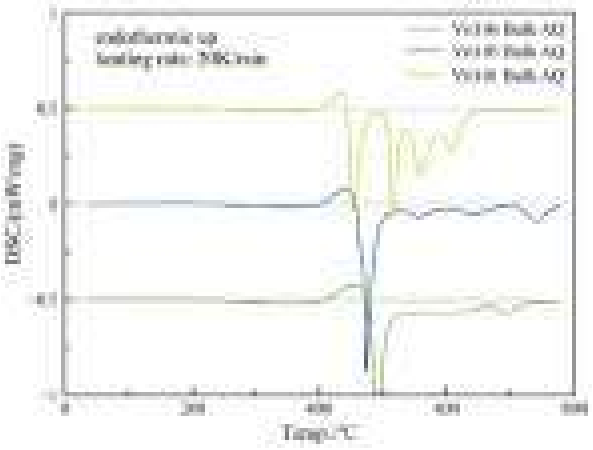

Fig. 2 DSC of metallic glass Vit101, Vit105 and Vit106.

In addition, SEM/EDS graphs of three kinds of metallic glasses also have been taken. In the future, we will discuss what changes had happened after T_x and try to know structural inhomogeneity inside these three kinds of metallic glasses.

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Keywords: Metallic Glass, Structural
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Effects of Mn on liquid metal embrittlement of Zn-coated steels

Galvanized steel is used to inhibit surface oxidation during heating, but the low melting point of Zn leads to the Zn-induced Liquid Metal Embrittlement (Zn-LME), where liquid zinc penetrates the grain boundaries of the steel during high temperature deformation and causes embrittlement. In this study, we focused on the effect of alloying elements on liquid metal embrittlement caused by zinc. The microstructure near the zinc / steel interface will be investigated after various heat treatments to clarify the effect of the alloying effects on the surface reaction.

Zn-LME phenomenon is more conspicuous in the higher Mn content. As the increasing of Mn content in the steel, the strength and ductility up to fracture of the Zn-coated specimens are rapidly reduced, and the fractured type also shown as brittle fractures [1, 2].

To identify the effect of Mn on Zn-LME, Fe-Mn binary alloys containing 9, 17, and 24 mass% (9, 17, 24Mn) were prepared. Each alloy was homogenized at 1150 °C for 24 hours and then rolled at 500 °C with a reduction of 50%, then annealed at 900 °C for 30 minutes. Fig.1 shows the EBSD map images of Fe-Mn alloys after annealing. The prior austenite grain sizes (PAGS) are 44, 58, and 52 μm, respectively, in the order of 9, 17, and 24Mn. Microstructure of the 9Mn is consist of the α'-Fe. 17 and 25Mn are composed with γ and ε-Fe. But all three alloys exist in the γ phase at temperatures where LME predominantly occurs (750-950 °C). [3, 4]

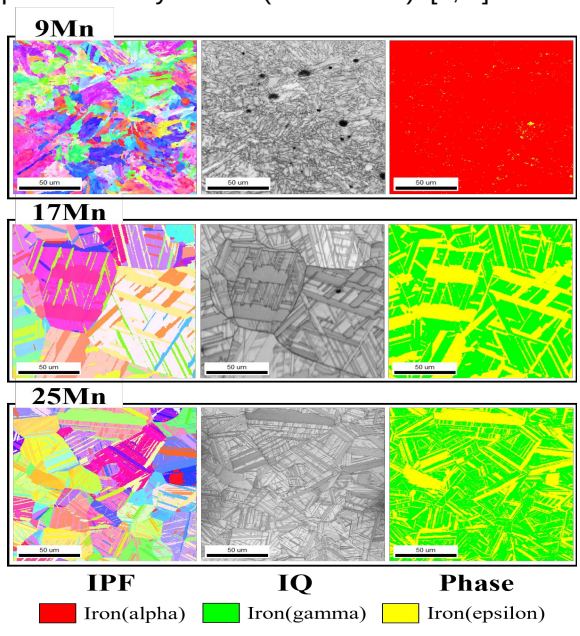

Fig. 1 EBSD inverse pole figure, Image quality, phase map images of Fe-Mn alloys after annealing.

Prior to experiments using Fe-Mn alloy, suitable conditions for electroplating and high temperature tensile test were investigated using pure iron. It was calculated that the Zn plating efficiency on Fe-Mn alloy was lowered by about 13% when using the same conditions as for pure iron. Fig.2 indicates the strain-stress curves of pure iron plated with 20 μm of Zn and bare specimens tensile tested at 850 °C, where the temperature at which LME is most intensified. The results clearly show lower mechanical properties in Zn plated specimen than those without due to the Zn-LME.

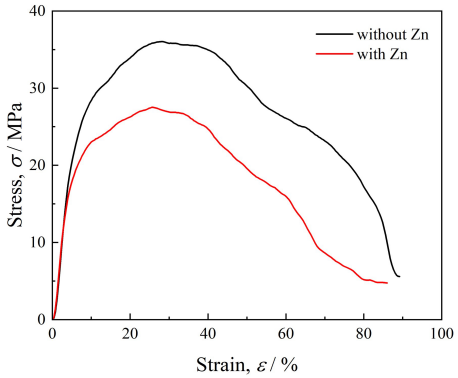

Fig. 2 Strain-Stress curves of pure iron specimens with or without Zn plating tensile tested at 850 °C.

High-temperature tensile tests and microstructural changes in Zn plated Fe-Mn alloys will be investigated using the conditions obtained in previous studies using pure iron.

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Development of conductive organic polymers containing carboxylate-bridged paddlewheel diruthenium(II,II) units

Abstract: Paddlewheel-type diruthenium complex exhibits interesting electronic properties because of the metal-metal interaction. In this work, poly(3,4-ethylene dioxythiophene)(PEDOT), which has the ability to conduct ions and electrons, was combined with paddlewheel diruthenium(II,II) units to synthesize conductive organic polymer. This diruthenium complex has great potential for applications in electrochemistry or organocatalysis.

The paddlewheel-type binuclear complexes with various metal centers have been widely studied in the past decades due to their distinctive structure.[1]

One of the most intriguing characteristics of paddlewheel complexes is their excellent redox-active properties: when oxidation and reduction of the two metal centers of the complexes occur, the metal-metal bond length changes systematically with the electronic arrangement of the frontier orbital $\sigma\pi_2\delta\delta^*\pi^*_2\sigma^*$, without significant structural changes[2]. Since $[Ru_2(OAc)_4]Cl$ was first synthesized by Stephenson and Wilkinson in 1966[3], numerous studies on the electronic properties, magnetic properties, and catalytic activities of paddlewheel diruthenium compounds have been published. This is mainly owing to the electronic configuration of the oxidation state $[Ru_2^{II,III}]$, which has a molecular orbital of $\sigma_2\pi_4\delta_2\pi^*_2\sigma^*$ (S=3/2), where the π* and σ* orbitals are nearly degenerated to make the oxidation state stable. Kojima and co-workers introduced amide- or carboxylate-based ligands to construct chiral paddlewheel diruthenium complexes, which exhibit remarkable catalytic properties and robustness in asymmetric C-C and C-N bond formation reactions[4]. Our group also combined $[Ru_2^{II,II}]$ with 7,7,8,8-tetracyano- p-quinodimethane (TCNQ) and its derivatives to design electron donor (D) and acceptor (A) metal-organic frameworks (MOFs), which exhibited switchable magnetism by external stimuli [2]. Although there are many studies on the $[Ru_2^{II,II}]$ linked with various types of ligands, the addition of highly conductive groups to $[Ru_2^{II,II}]$ has not yet been investigated, particularly in light of their catalytic properties.

Poly(3,4-ethylene dioxythiophene)(PEDOT) is one of the conducting polymers which has chemical stability, dynamic electrochromic activity, and biocompatibility[5]. In recent years, PEDOT has been studied for applications such as biosensors, organic light-emitting diodes, and energy conversion and storage [6]. If the highly conductive PEDOT is chemically bonded to the paddlewheel diruthenium with redox activity, it is possible to obtain a chemically active conductive organic polymer with high catalytic performance (Fig. 1).

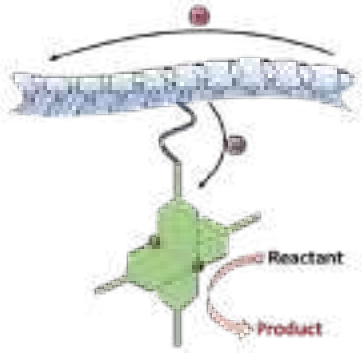

Fig. 1 Schematic illustration of $[Ru_2^{II,II}]$-PEDOT complex.

In this work, we have synthesized for the first time paddlewheel diruthenium compounds $[Ru_2(CHOphCO_2)_4(THF)_2]$ containing aldehyde groups in four directions and determined their structures by IR, single crystal single-crystal X-ray diffraction (XRD), and other characterizations. The aminated EDOT monomer was linked to the aldehyde group of $[Ru_2^{II,II}]$ by an aldimine condensation reaction to form the complex **1**, where the formation of C=N bonds was confirmed by IR and other characterizations. To obtain high conductivity based on complex **1**, the polymerization of EDOT should be involved. Thus, the EDOT on complex **1** was polymerized (Fig. 1) by the post-polymerization method, in which the polymerized **1** displays the redox activity and high conductivity in a single material. This work might provide new ideas for the application of paddlewheel diruthenium(II,II) units in fields such as electrocatalysis. Related work is in progress.

Keywords: Polymer, Catalytic
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Processing of micro-porous metallic powders by liquid metal dealloying

This project aims to apply liquid metal dealloying to metal powders and is motivated both by the limits of dealloying on massive materials and by the applications that microporous powders could make possible. The use of this process on powders targets a better control of their porosity, in order to tune their mechanical properties and to allow their use in additive manufacturing techniques.

Introduction

Additive manufacturing techniques are getting more and more widespread, allowing the development of architectural materials with exceptional functional or mechanical properties. Powders are the key ingredient of metallic additive manufacturing, and the study and modification of their properties is therefore essential to improve these new manufacturing processes. This project aims to develop porous metal powders via liquid metal dealloying [1].

From elaborating powders to predicting their morphology using computer simulation, this stay in Tohoku University had several objectives that will be detailed below.

Etching dealloyed commercial powders

The first part of this project consisted in etching and analyzing dealloyed commercial powders (Invar and Inconel 718) elaborated in France. Porous powders were successfully obtained (Fig. 1) and open new avenues to explore their potential as ingredients in additive manufacturing. Moreover, extensive microscopic characterization enabled to detect phases appearing for the first time in the dealloying process such as MgNi2.

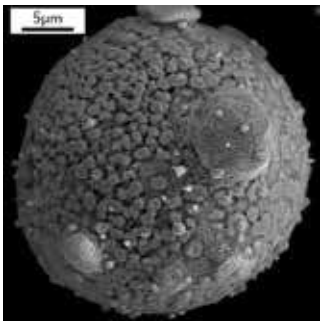

Figure 1: Porous FeCr powder

Elaborating powders with controlled compositions

After the study about commercial alloys, this stay enabled to manufacture powders with a controlled position, thanks to the knowledge and the equipment of Kato Laboratory. Hence, using an atomization tower, several grades of FeMgNi and AgCuNi powders could be manufactured. These grades will enable a comparison between commercial and model alloys, as well as facilitating the understanding of the dealloying process as they do not contain much alloying elements.

Predicting powders morphology

The last part of this project consisted in developing a numerical model for predicting dealloying kinetics and morphologies, in order to optimize the manufacturing parameters. Hence, a 1D model based on diffusion was developed and showed results in semi-quantitative agreements with the experiments for CuNi dealloyed powders (Fig. 2) and is yet to be adapted to FeNi powders.

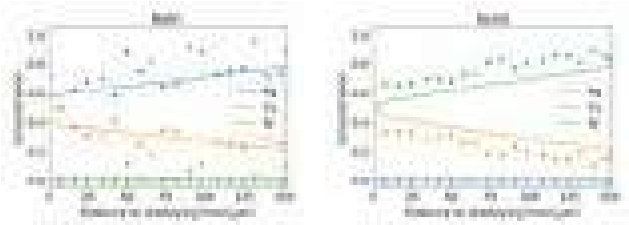

Figure 2: Cu50Ni50, 1273K – experimental and simulated composition profiles for the bath (left) and ligaments (right)

Conclusion

This stay in Tohoku University opens new ways for a better understanding of the dealloying process and allowed to define a complete process to elaborate porous powders that are expected to be mechanically characterized and used for additive manufacturing in a near future.

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