

# ICC-IMR FY2019 Activity Report

http://www.icc-imr.imr.tohoku.ac.jp/

# ICC-IMR FY2019 Activity Report

### **International Collaboration Center**

Institute for Materials Research Tohoku University

# CONTENTS

Mission
Committee Members ······03
Visiting Scholars05
Workshops ······23
Young Researcher Fellowships · · · · · · · · · · · · · · · · · · ·



# 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 65 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.



USA 100
China 90
Germany 85
France 77
Korea 63
UK 39
Russia 26
Netherlands 22
Switzerland 16
India —— 14
Poland 13
Australia 10
Canada 10

Taiwan 10
Singapore 8
Spain 8
■ Iran 7
Thailand 6
Denmark 5
Hong-Kong 5
Norway 5
Mexico — 4
Czech Republic 3
Italy 3
Slovakia 3
Belgium 2

Rumania	2
Slovenia	2
Ukraine	2
Austria	2
Argentina	1
Brazil	1
Egypt	1
Indonesia	1
Serbia	1
Sweden	1
Turkey	1
Vietnam	1

# ICC-IMR COMMITTEE MEMBERS

Director

Prof. Gerrit E. W. BAUER

Steering Committee

Prof. Hidemi KATO

Prof. Hiroyuki NOJIRI

Prof. Hitoshi MIYASAKA

Prof. Akira YOSHIKAWA

Prof. Masaki FUJITA

Prof. Yoshinori ONOSE

Prof. Dai AOKI

Prof. Kozo FUJIWARA

# Activity Report

Visiting Scholars

# **Visiting Scholars**

Application No.	Title in IMR	Name	Affiliation	Host Professor	Proposed Research	Term
19G01	Visiting Associate Professor	Ruihua He	Westlake University, China	Prof. Fujita	Search for Materials with 3D Negative Electron Compressibility	2019.5.23-6.27
19G02	Visiting Assistant Professor	llya Okulov	The University of Bremen, Germany	Prof. Kato	Establishing a Hybrid Manufacturing Technology Combining Liquid Metal Dealloying and Additive Manufacturing for Production of Functional Nanoporous Materials	2019.5.8-2019.6.7
19G03	Visiting Professor	Deng Pan	MGI, Shanghai University, China	Prof. Chiba	Processing-Dependence of Mechanical Properties and Governing Deformation Mechanisms of Ti-Nb Alloys by Additive Manufacturing	2019.6.3-2019.8.30
19G04	Visiting Associate Professor	Subhankar Bedanta	National Institute of Science Education and Research (NISER), India	Prof. Takanashi	Spin Pumping in Bi <sub>2</sub> Se <sub>3</sub> (MoS <sub>2</sub> )/CFMS Layers	2019.6.17-2019.7.26
19G05	Visiting Professor	Jiang Xiao	Fudan University, China	Prof. Bauer	Spin Cavitronics	2019.8.1-2019.8.31
19G06	Visiting Professor	IIya Sheikin	LNCMI, CNRS, France	Prof. Aoki	Superconductivity, Quantum Phase Transitions and Fermi Surface of Strongly Correlated <i>f</i> -Electron Systems	2019.7.1-9.30
19G07	Visiting Assistant Professor	Ivan Soldatov	Leibniz Institute for Solid State and Materials Research, Dresden, Germany	Prof. Takanashi	Magnetic Domain Imaging of Ferromagnetic Thin Films	2020.2.3-2020.3.19
19G08	Visiting Professor	Hyoung Seop Kim	Pohang University of Science and Technology, Korea	Prof. Kato	Ultrafine Grained Materials, High-Entropy Alloy	2019.12.23-2020.1.31

#### Collaborations on ARPES study of quantum materials

Here I summarize my activities during my visit to ICC-IMR as a visiting associate professor hosted by Prof. Masaki Fujita. In particular, I briefly describe two projects in ongoing collaboration with the Fujita group on ARPES study of quantum materials, i.e., 3D negative electronic compressibility in electron-doped cuprate superconductors, and doping dependence ARPES study of complex oxides based on vacuum annealing.

During my visit to ICC-IMR as a visiting associate professor, I had the opportunity to do the following things: to work closely with Prof. Masaki Fujita's group; to visit Prof. Y. Koike's group, Prof. T. Sato's lab and Prof. H. Kumigashira's group; to visit the synchrotron lightsource UVSOR at the Institute for Molecular Science in Myodaiji, Okazaki; to attend the 12th International Conference on Spectroscopies in Novel Superconductors (SNS2019) at University of Tokyo. In particular, through numerous face-to-face discussions with various members of the Fujita group, exchanges of ideas were very effective and a few projects for collaborations based mainly on ARPES measurements were identified. I will briefly summarize two of them in the following.

**Project 1:** 3D Negative electronic compressibility (NEC) in electron-doped cuprate superconductors.

My previous group at Boston College found with ARPES in an iridate material Sr3Ir2O7 first evidence for 3D NEC [1], which is a new emergent phenomenon driven by strong electron correlations. This finding points to a distinct pathway towards an uncharted territory of NEC featuring bulk correlated metals with unique potential for applications in low-power nanoelectronics and novel metamaterials beyond reach of their 2D cousins [2].

Preliminary evidence obtained by my current group suggests the occurrence of NEC electron-doped cuprates in Nd2-xSrxCuO4 (NCCO) at 0.04≤x≤0.10 and its crossover onto a positive electronic compressibility (PEC) regime at higher doping levels (Fig. 1a-b). Consistent with this preliminary experimental result, single-band Hubbard model calculation performed by Prof. A. Bansil's group at Northeastern Univ. obtains a NEC phase which crosses over into PEC beyond a boundary dependent of the tight-binding band structure parameters and doping level (Fig. 1c). According to the calculation, NEC in this system is driven by the antiferromagnetic correlations (tunable

by an effective on-site Coulomb repulsion in the calculation) which are strongly weakened with increasing electron doping, reminiscent of the case of Sr3lr2O7 [3]; the NEC-PEC crossover occurs as these correlations become too weak and the valence band crosses the Fermi level forming hole pockets that tend to drive the chemical potential up.

If confirmed, these results would constitute the first experimental case of NEC in cuprates that had eluded early observation. It would also constitute the first case of NEC-PEC crossover in a bulk metal, which occurs between two metallic phases. We plan to perform an integrative study to scrutinize these results, in terms of the deep valence band and core level shifts and low-energy band structure based on both bulk Ce and surface K doping. Combining both doping approaches allows to assess the role of disorders in connection with the recent controversy about the effect of annealing condition on the electronic properties of electron-doped cuprates.

Related to this project, the Fujita group has provided samples of NCCO as well as PrLa0.6CexCuO4-d for a comparative study.

**Project 2:** Doping dependence ARPES study of complex oxides based on vacuum annealing.

We are in the process of developing a new experimental technique in order to obtain entire doping evolution of materials electronic structure on a given cleaved surface without the need of changing samples as in most traditional doping dependence studies.

The idea of this capability is derived from Ref. [4], which showed that sample surface after can survive repeated vacuum and ARPES data annealings, quality remained good after one month's repeated treatments and measurements. The authors did their sample annealing in a MBE chamber with a poor vacuum, and the

### Visiting Scholars

treatment process involved multiple sample transfers; these two factors tend to reduce the sample surface lifetime. Besides, the quenching mechanism was largely absent, except when the sample is transferred from the MBE chamber after fresh annealing back onto the liquid-helium cryostat--a "slow" process that would take ~10 mins.

We intend to perform vacuum annealing & quenching of samples in the same chamber where ARPES measurements are carried out. The procedure is as follows: First, laser heating a given cleaved surface of single-crystal sample up to 1300 C for a few seconds/mins, then remove the laser and the sample will be quenched instantly as the sample has been sitting on the liquid helium cryostat during the entire treatment. Each of such a treatment cycle can alter the oxygen content of the sample surface which is then subject to subsequent ARPES measurement.

In light of the potentially substantial improvements in our design, our treatment process should offer a much cleaner, efficient and effective way to tune (decrease) the sample surface oxygen content in-situ. The dream experiment in pursuit with this new technique is to study quantum criticality in ARPES, which requires finetuning of doping level and measurement with high precision and reproducibility --challenges that have prevented the use of advanced experimental techniques other than transport measurements for the quantum criticality research, although those transport studies were already quite impactful.

Related to this project, the Fujita group has provided hole-doped cuprate superconductor Bi2Sr2CuO6+x samples [5] for the ongoing testing required for our new experiment technique.



Fig.1 Doping dependence of the (**a**) spectra (second derivative) at  $\Gamma$  and (**b**) dispersion along a momentum cut through  $\Gamma$  of two deep valence bands on Nd2-xCexCuO4 at 70 K. (**c**) Hubbard model calculation of the chemical potential as functions of x and the ratio between next-and nearest-neighbor hopping parameters.

#### <u>References</u>

[1] J. He et al., Nature Mater. 14, 577-582 (2015).

[2] W. Wen et al., J. Supercond. Nov. Magn, 33, 229-239 (2020).

[3] J. L. Schmehr et al., Phys. Rev. Lett. 122, 157201 (2019).

[4] Y.-G. Zhong et al., Phys. Rev. B 98, 140507(R) (2018).
[5] G. Yu et al., Phys. Rev. B 99, 214502 (2019).

Keywords: photoemission, electronic structure, superconducting Ruihua He (Westlake University) E-mail: heruihua@westlake.edu.cn

# Hierarchical nanoporous material by liquid metal dealloying of additively manufactured precursor

Nanoporous materials possessing large surface area and high electrical conductivity demonstrated advantages for various energy applications. The efficiency of these materials would be greatly improved through creating regular microscale channels for improved mass transport. Here, we propose an approach for the synthesis of nanoporous materials with regular microscale channels via a combination of additive manufacturing and liquid metal dealloying.

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

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

In this work, Inconel 718 alloy was selected for dealloying in liquid magnesium. The Inconel 718 mainly consists of Ni, Fe, Cr, Nb, and Ti elements. The heat of mixing  $\Delta Hmix$ between Mg and Ni is negative. The heat of mixing  $\Delta Hmix$  between Mg and each of the remaining elements is positive. Therefore, Ni will be dissolved into Mg during liquid metal dealloying. The remaining elements will be rejected by liquid magnesium and rearranged into an open porous structure.

The Inconel 718 samples consisting of strut structures and having regular porous channels were additively manufactured using a commercial selective laser melting set-up (Figure 1). Thereafter, the samples were subjected to liquid metal dealloying, namely immersed in liquid magnesium, to create nanoscale porosity in the strut structures. After dealloying, the evolved nanoscale pores were filled with magnesium. Magnesium was removed by chemical etching of the samples in 3M aqueous solution of nitric acid. Finally, the hierarchical porous samples were obtained.

Figure 2 shows the microstructure of the Inconel 718 samples struts after liquid metal dealloying. According to the microstructural analysis, the struts mainly consist of two nanoscale phases. These are FeCrNbTi-based and Mg-based phases. It has to be emphasized that the typical for the selective laser melting melt pool profiles remained after dealloying and are clearly distinguished as a bright contrast in the form of thin lines (Figure 2).



Fig. 1 shows additively manufactured Inconel 718 samples

The chemical etching of the dealloyed samples resulted in the formation of an open porous ligament structure typical for liquid metal dealloying. The size of ligaments is a few tens of nanometers (Figure 2). This is comparable with that of the recently reported nanoporous high-entropy alloys [2] and two orders of magnitude smaller as compared with the ligament size of

### **Visiting Scholars**

dealloying-based porous Fe [3].

The hierarchical porous material synthesized in this study implies advantages for both functional and structural applications. In the case of functional applications, large pores enable efficient mass transport and small pores provide a high surface area. In the case of structural applications, the yield strength of the nanoscale ligaments typically reaches the theoretical strength of the material [2]. Thus, together with the low sample density due to a high fraction of pores, the hierarchical porous samples might possess significantly improved specific strength characteristics.

#### **References**

[1] T. Wada, K. Yubuta, A. Inoue and H. Kato, Mater. Lett.
65 (2011).

[2] S.-H. Joo et al. Adv. Mater. 6 (2020).[3] I.V. Okulov et al. Scripta. Mater. 163 (2019).



Fig. 2 Microstructure of additively manufactured Inconel 718 sample after liquid metal dealloying: (a) Joining of sample struts, (b-c) Melting pool profiles (bright lines), (d) Multiphase microstructure, and (e) Nanoporous structure after chemical etching of dealloyed samples

Keywords: Porosity

Soo-Hyun Joo and Hidemi Kato (Institute for Materials Research, Tohoku University, Japan) E-mail: <u>okulovilya@gmail.com</u>

http://www.imr.tohoku.ac.jp/index.html

Ilya Okulov (Institute for Materials Research, Tohoku University, Japan; Institute of Natural Sciences and Mathematics, Ural Federal University, Russia; University of Bremen, Germany; and Leibniz Institute for Materials Engineering, Germany)

Lutz Mädler (University of Bremen, Germany and Leibniz Institute for Materials Engineering, Germany) Stanislav Evlashin (Skolkovo Institute of Science and Technology, Russia)

# Data-driven Design of Rhenium-free Ni-based Superalloy and its Additive Manufacturing by an Electron Beam

Introductory part, Abstract: A state-of-the-art trend in developing superalloys with high performance and low cost is to avoid the use of elements such as rhenium and ruthenium whereas sustaining desirable high-temperature mechanical properties. Based on the philosophy of materials genome engineering and our previous work, this collaborative research is to establish a methodology of data-driven design of one Rhenium-free Nickel-based superalloy and its additive manufacturing by electron beam.

From June to August in 2019, Prof. Deng Pan from Shanghai University visited Prof. Akihiko Chiba group to further their collaboration on development of advanced metallic materials and their applications by electron beam additive manufacturing (EB-AM). To be more specific, the two groups aims at developing a methodology of data-driven design of a superalloy processed by EB-AM. During his stay, Prof. Pan worked closely with Prof. Chiba and his group members including Drs. Huakang Bian and Qisheng Li, Mr. Lingxiao Ouyang on development of relevant techniques such as high-throughput fabrication and processing of alloy powders. As a result of this visit, two collaborative proposals have been successfully submitted to National Science Foundation of China (NSFC) and Japan Science Promotion Society (JSPS), respectively, in 2020.

Nickel-based superalloys (NBS) contain carefully balanced alloying additions of chromium, cobalt, aluminium, titanium and other elements and have been widely used in applications of turbine blades in air turbine engines for power generation, aircraft and marine propulsion.

It is well known that use of rhenium in the NBS greatly improves the creep resistance at high temperatures, hence the in-service temperature, of the alloy. However, formation of topological close-packed phases (TCP) in company of the rhenium addition in the NBS embrittles the superalloy at room temperature. In addition, sparse reserves as well as high cost of alloying elements such as rhenium and ruthenium significantly hinder their potential in material selection for future designs of turbine engine components. In consequence, a state-of-the-art trend in developing alloys with a combination of high performance and low cost for turbine blades is to avoid the use of elements such as rhenium and ruthenium whereas sustaining desirable high-temperature mechanical properties such as superior creep resistance and excellent oxidation resistance. Moreover, availability of performance evaluation and properties data of the alloys are of essential importance to ensure the reliability of turbine engines. Nevertheless, conventional 'trial & error' approach appears to slow down the progress in search of more advanced NBS as a result of the complexity in alloy composition and extremely long and costly design cycles.

The philosophy of Materials Genome Initiative (MGI) first proposed by Barack Obama in 2012 has been widely implemented in recent years to accelerate the discovery, design, development and deployment of new, advanced materials by employing high-throughput computational selection, machine learning and high-throughput synthesis/characterization techniques. For example, Liu et al designed an amorphous alloy system (Ir-Ni-Ta-(B)) with a glass transition temperature of 1162K and strength of 3.7GPa at 1000K by high-throughput MGI engineering, which significantly improves the properties of other bulk metallic glasses and conventional high-temperature alloys [1].

Additive manufacturing (AM) is defined as the process of joining materials to make parts from 3D model data, usually layer upon layer, as opposed to subtractive and formative manufacturing methodologies became а research highlight in the world in recent years. Electron beam melting (EBM) as one AM technology have been used in aerospace and medical fields because EBM can produce the product directly with complex shapes and excellent quality materials. The interest of industry in EBM technology is increasing year by year.

By in-depth discussions and preliminary efforts by Prof. Pan and Chiba group, a few key scientific and technological issues have been sorted out for successful implementation of this joint research:

i) the strengthening mechanism(s) by solid solutions in the complex and multicomponent superalloys without Rhenium addition, which may be hinged to a) the interaction among alloying elements in the multicomponent alloy, and b) the interaction between the alloying elements and defects such as dislocations and stacking faults.

### Visiting Scholars

ii) The phase transformation in solid-liquid and liquid-liquid interfaces during melting and solidification processes of Rhenium-free superalloy by electron beam 3D printing.

iii) High temperature measurements of mechanical properties of small-sized superalloys.4. to optimize the reversed design parameters (processing windows) for one material and fast yet reliable microstructural characterization during electron beam 3D printing.

In turn, combination of first principle calculations and machine learning, machine learning prediction models of substitutional energy of alloying elements will be established and trained for prediction of substitutional energy and local geometry of NBS and the occupying tendency of alloying elements in multicomponent system: a) different elements in the same phase ( $\gamma or \gamma'$ ); and the same element in different phases ( $\gamma and \gamma'$ ); b) different elements in the same defect (dislocation or stacking fault); and the same element in different defects (dislocation and stacking fault); c) the same element in different phases and defects; d) microstructural and stoichiometric analysis of model alloys.

More than 10 compositions will be expectedly proposed for fabrication of alloy powders by casting followed by atomization for 3D printing. Millimeter-sized specimens will consequently be produced by 3D printing, the processing parameters of which will be rapidly and effectively optimized employing in-house high-throughput technique of single-channel electron beam melting (3-5 scanning for each of 5\*5 specimens) (Fig. 1) and machine learning prediction.

The temperature-dependent mechanical properties (e.g. elastic modulus, yield strength, creep) of the small-sized specimens will be characterized by high temperature microsample uniaxial tensile testing and stress relaxation with a designed temperature range from ambient to

900 °C. The strain measurement of tiny specimens is implemented via a non-contact interferometric technique based on Young's two-slit interference principle. The reliability, accuracy and effectiveness of the resulting data-mining and artificial intelligence paradigm will be validated and optimized.



Fig.1 shows a high-throughput electron-beam additive manufacturing technique at Chiba group for batch fabrication and processing optimization of small size samples.

#### **References**

[1] Li MX, Zhao SF, Lu Z, et al. Nature (2019), 569(7754): 99.

Keywords: alloy, powder processing Deng Pan (Materials Genome Institute, Shanghai University, China) E-mail: DPan\_MGI@shu.edu.cn http://mgi.shu.edu.cn/

#### Spin Pumping in Bi<sub>2</sub>Se<sub>3</sub> (MoS<sub>2</sub>)/CFMS Layers

One of the effective ways for conversion of charge (spin) current to spin (charge) current is to exploit spin Hall effect (inverse spin Hall effect), which is the vital of recent spintronic applications. In this project, our aim is to prepare Heusler alloy based  $Co_2Fe_xMn_{1-x}Si$  (CFMS) films on top of topological insulator  $Bi_2Se_3$  and 2-dimensional chalcogenide  $MoS_2$  films in order to understand the conversion mechanism between the Heusler alloy and the nonmagnetic materials. As the first step, we investigated the growth condition of those nonmagnetic materials and the spin pumping from the Heusler alloy.

The generation and control of spin current, which is the flow of spin angular momentum, are for the important research subjects contemporary spintronics. Spin current-based memory and storage devices are predicted to be faster, power efficient compared to spin polarized current devices [1]. One of the ways to convert from charge (spin) current to pure spin (charge) current is called spin Hall effect (inverse spin Hall effect). In the case of bilayer systems consisting of ferromagnetic (FM) layer and nonmagnetic (NM) layer, the conversion efficiency majorly depends on spin-orbit coupling strength of NM. For the spin pumping experiment, the FM layer works as a spin current source, where spins dissipate their spin angular momentum at the interfaces between the FM layer and the NM layer. As the NM material, the elemental heavy metals such as Pt, W, Ta, and Au are to investigate the spin pumping via ISHE [2].

Apart from the NM metals, topological materials and 2-dimensional chalcogenides have attracted much attention as materials for the spin-charge conversion. From this point of view,  $Bi_2Se_3$  and  $MoS_2$  are the potential candidates due to presence of spin momentum locking surface states and absence of inversion symmetry, respectively [3]. Therefore, it is indispensable to elucidate the spin-charge conversion mechanism in those topological materials and 2-dimensional chalcogenides for realizing next-generation spintronic devices.

In addition to the NM material exhibiting the high spin-charge conversion efficiency, the fast and low power consumption spintronic devices require the FM layer materials with low magnetic damping constant ( $\alpha$ ). In this context, Heusler alloys viz. Co<sub>2</sub>Fe<sub>x</sub>Mn<sub>1-x</sub>Si (CFMS) are promising FM layer material showing the small value of  $\alpha \sim$ 0.002, which is one order of magnitude lower than those for the conventional FM materials such as a FeNi alloy (Permalloy). Some of Heusler alloys are also famous as a half metal theoretically predicted, which may allow us to create highly spin-polarized current. Considering the above points, the Heusler alloys and the topological materials or the 2-dimensional chalcogenides are important materials combination as a bilayer system for spin

pumping experiment.

In this collaborative research, we proposed the investigations of spin pumping by measuring inverse spin Hall effect (ISHE) in  $Bi_2Se_3$  (MoS<sub>2</sub>) / CFMS bilayers. As the first step, we prepared the  $Bi_2Se_3$  and MoS<sub>2</sub> thin films by electron beam evaporation, and investigated the spin pumping from the CFMS using the bilayer with CFMS and Pt layers.

Figure 1 shows the x-ray diffraction data for a 30 nm Bi<sub>2</sub>Se<sub>3</sub> film deposited on Si (100) substrate. It shows the diffraction peaks corresponding to (003) family of planes of Transmission orientation only. electron microscopy confirmed the polycrystalline nature films We have the [4]. observed of magnetoresistance of ~ 7% in  $Bi_2Se_3$  thin films. Similarly, we have prepared MoS2 films by electron beam evaporation. The thickness of MoS<sub>2</sub> films are kept about 10 nm to make sure the film is uniform and homogeneous. Raman scattering data indicate the MoS<sub>2</sub> phase formation of the films. We have observed spin pumping and invserse spin Hall effect in MoS<sub>2</sub>/CoFeB bilayers which evidence that the MoS<sub>2</sub> exhibit high spin orbit coupling.



Fig. 1 X-ray diffraction profile of a 30nm  $Bi_2Se_3$  film grown on the Si substrate measured in the  $\theta$ -2 $\theta$  geometry.

### Visiting Scholars

In addition to the investigation of film growth, we analyzed the ISHE voltage and damping results on CFMS (20 nm) / Pt (t) bilayers, where t was varied between 3 to 20 nm. On these bilayers, we performed the ferromagnetic resonance (FMR) measurement in the frequency range of 6 to 17 GHz. As a result, we observed the enhancement of damping for the samples attached with Pt, which is attributable to the large spin-orbit interaction of Pt. In order to confirm the spin injection originating from the spin pumping, we performed angle dependence measurement for the ISHE voltage. We did further analysis to disentangle the spin pumping voltage from other spin rectification effects such as anisotropic magnetoresistance, anomalous Hall effect. We found spin pumping voltage is dominating in our CFMS / Pt bilayers.

We have also performed analysis to quantify the spin mixing conductance, which is an important parameter corresponding to the ferromagnetic material. Figure 2 shows the spin mixing conductance as a function of Pt layer thickness. We show that CFMS exhibits a very high spin mixing conductance of 1.77 X 10<sup>20</sup> m<sup>-2</sup>. Furthermore, we have analyzed the interface transparency, which was evaluated to be 84% for CFMS / Pt system. This value is higher than the values reported for other ferromagnetic / heavy metal systems [5]. Our study shows that CFMS is an ideal FM layer for spin-charge conversionbased applications. We plan to deposit CFMS film on Bi<sub>2</sub>Se<sub>3</sub> and MoS<sub>2</sub> and investigate the spin pumping for those bilayers in near future.



Fig. 2 Spin mixing conductance as a function of Pt layer thickness for the CFMS (20 nm) / Pt bilayers.

Keywords: Half metal, ferromagnetic, thin films Dr. Subhankar Bedanta (NISER-Bhubaneswar, India) E-mail: sbedanta@niser.ac.in http://sbedanta.wixsite.com/niser

#### **References**

[1] F. Hellman, Rev. Mod. Phys. 89, 025006 (2017).

[2] A. Hoffman, IEEE Trans. Magn. 49, 5172-5192 (2013).

[3] M. Z. Hasan, et al., Rev. Mod. Phys. 82, 3045 (2010).

[4] B. B. Singh *et al*, *Phys. Stat. Sol.: Rap. Res. Lett.*, 1800492 (2018).

[5] B. B. Singh, K. Roy, P. Gupta, T. Seki, K. Takanashi, and S. Bedanta (submitted).

#### Realizing Hopfield Network by Magnetic Textures

We propose that the mutual interaction between a magnetic texture and an electric current leads to a self-adaptive behavior of the whole system, which can be used to construct an artificial neural network such as the Hopfield network, realizing an associate memory. Different from other approaches, here the learning rules are naturally imbedded in the physical system.

Neuromorphic computing, brainor inspired computing receives inspiration from the human brain, which is both powerful and extremely energy efficient. The Artificial Neural Network (ANN) is a prime model to mimic the working mechanism of the brain. An ANN consists of a pool of simple (neurons) processing units that communicate with each other by means of a large number of weighted connections. Such a model has already been successfully implemented into algorithms and is widely used in facial/vocal recognition, pattern classification etc. However, most industry-level algorithms are running on conventional digital computers. Due to the drawbacks of classical computers (such as Joule heating and the von-Neumann the bottleneck), realizations of these algorithms are energy inefficient. One solution of this issue is to customize chips for ANN algorithms, or to build a hardware ANN.

Spintronics offers opportunities for this evolution [1]. For example, Spin Torque Nano Oscillators based on Magnetic Tunnel Junctions (MTJs) have been used as "spintronic neurons" to implement simple classification tasks [2,3]. Here we demonstrate that the magnetic system with adaptive magnetic textures offers a platform for neuromorphic computing. In a uniform film, the internal magnetic textures give rise to a rich degree of freedom. Due to Anisotropic MagnetoResistance the (AMR) [4,5], the electric conductance depends on the local magnetization, which induces a nonuniform electric current distribution in the presence of a voltage bias. On the other hand, the magnetic texture can be modified by electric currents via the current-induced spin transfer torque (STT).

Fig.1 (a)-(d) shows the time revolution of a magnetic stripe texture (black and white color for magnetization pointing out-of and into the paper) with applied voltage from the top to the bottom edge. Due to the current-induced spin transfer torque, the stripes tend to align perpendicularly to the current direction. The evolving texture leads to a change in the electric conductance due to the AMR. Therefore, with current applied on vertical direction, the vertical



conductance increases while the horizontal one decreases, indicating that the mutual interaction between a magnetic texture and the electric current leads to a self-adaptive behavior of the whole system. By interpreting the voltage on each node as input, and electric current flowing into/out of the node as output, the weight can be described by the electric conductance, which is a matrix when there are multiple nodes. Therefore, the magnetic system can be used to construct an artificial neural network via a trainable conductance matrix.

### **Visiting Scholars**



Fig. 2 Proof of principle for a Hopfield network with 7 nodes mimicking the configuration of IMR logo. (a) Current distribution during the learning process, where the nodes are applied with voltages  $V=V_0\{1,-1,1,-1,1,-1,1\}$ . (b) The configuration of magnetic texture when the learning process is finished.

Fig. 2 demonstrates the proof-of-principle structure for a network composed of 7 nodes. In this configuration, all nodes are treated as input and output at the same time. This is therefore a Hopfield network that can be used as an associative memory. By applying a voltage to each node, the current will be distributed according to Kirchhoff's law and drive the magnetic texture accordingly. When the texture reaches a stable configuration, the learning process is finished. The information about the weight matrix can be extracted by measuring the conductances, realizing the function of an associative memory, i.e. the pattern we input to the network can be recognized again even if we input a wrong pattern.

In conclusion, we propose a self-adaptive magnetic system that can be used to perform neuromorphic computing. In contrast to competing setups, the learning process in this setup (or the learning rules) is naturally imbedded in the physical system.

#### **References**

- J. Grollier, D. Querlioz, K. Y. Camsari, K. Everschor-Sitte, S. Fukami, and M. D. Stiles, Nature Electronics 1 (2020).
- [2] M. Romera, P. Talatchian, S. Tsunegi, F. A. Araujo, V. Cros, P. Bortolotti, J. Trastoy, K. Yakushiji, A. Fukushima, H. Kubota, S. Yuasa, M. Ernoult, D. Vodenicarevic, T. Hirtzlin, N. Locatelli, D. Querlioz, and J. Grollier, Nature 1 (2018).
- [3] A. Mizrahi, T. Hirtzlin, A. Fukushima, H. Kubota, S. Yuasa, J. Grollier, and D. Querlioz, Nature Communications 9, 1533 (2018).
- [4] D. Pinna, G. Bourianoff, and K. Everschor-Sitte, ArXiv:1811.12623 [Cond-Mat] (2018).
- [5] D. Prychynenko, M. Sitte, K. Litzius, B. Krüger, G. Bourianoff, M. Kläui, J. Sinova, and K. Everschor-Sitte, Phys. Rev. Applied 9, 014034 (2018).

Keywords: spintronic, magnetoresistance, spin current Prof. Jiang Xiao (Department of Physics, Fudan University, China) E-mail: xiaojiang@fudan.edu.cn

http://www.physics.fudan.edu.cn/tps/people/jxiao/

# Superconductivity, Quantum Phase Transitions and Fermi Surface of Strongly Correlated *f*-Electron Systems

This research project is built upon our long-standing, successful collaboration with Prof. D. Aoki. We have investigated two families of Ce-based heavy-fermion materials, in which quantum criticality can be induced by doping. To this end, several new samples were grown. Some of these studies yielded interesting preliminary results, and will be continued, also in high magnetic fields. In addition, we have finished the analysis and discussion of some of the previously obtained data. In conjunction with new results, this gave rise to two articles submitted to high-level journals. One of them was recently published [1].

Quantum critical points (QCPs), i.e., continuous phase transitions at zero temperature, play a key role in the physics of heavy-fermion (HF) compounds and other materials. Recent theoretical attempts to classify QCPs in HF systems rely on the knowledge of whether the f electrons are itinerant or localized on both sides of a QCP, i.e. whether or not they contribute to the Fermi surface (FS). This can be achieved by comparing experimentally established FS topology with the results of band structure calculations performed for both itinerant and localized f electrons. Magnetic quantum oscillations, such as the de Haas-van Alphen (dHvA) effect, are the most direct way to establish the FS topology of a metal.

CeRhIn<sub>5</sub> is one of the best-studied HF materials. This tetragonal antiferromagnetic (AFM) compound with  $T_{\rm N} = 3.8$  K can be tuned to a QCP by pressure, chemical substitution, and magnetic field. Several dHvA experiments evidence that the f electrons of CeRhIn<sub>5</sub> are localized at ambient pressure, although some of the theoretically predicted dHvA frequencies were not experimentally observed. As the critical pressure for the suppression of antiferromagnetism,  $P_{\rm c} = 2.3$  GPa, is reached, all dHvA frequencies observed at  $P < P_c$  change discontinuously, signaling an abrupt FS reconstruction as a consequence of the f-electron delocalization. In addition, the effective masses diverge at  $P_{\rm c}$ . A similar discontinuous change of the dHvA frequencies was observed upon substituting Rh by Co in CeRh<sub>1-x</sub>Co<sub>x</sub>In<sub>5</sub>. However, the FS reconstruction does not occur at the critical concentration  $x_c \approx 0.8$ , where the AFM order is suppressed, but deep inside the AFM state, at  $x \approx 0.4$ , where the AFM order alters its character and superconductivity emerges to coexist with antiferromagnetism. Furthermore, the effective masses do not diverge here.

Another way to tune CeRhIn<sub>5</sub> to quantum criticality is to substitute Rh by Ir [2], as shown in Fig. 1(a). Upon doping CeRhIn<sub>5</sub> with Ir, the antiferromagnetic order is suppressed at a critical concentration  $x_c = 0.6$  giving rise to a QCP. In addition, a commensurate magnetic order develops above the Ir concentration of about 0.3, and co-exists with the incommensurate structure up to  $x_c$ . Finally, superconductivity was observed over a wide concentration range 0.3 < x < 1.





The FSs and effective masses of the end compounds, CeRhIn<sub>5</sub> and CeIrIn<sub>5</sub>, are well known. CeRhIn<sub>5</sub> is characterized by FSs with localized felectrons and only slightly enhanced effective masses. On the contrary, CeIrIn<sub>5</sub> posses Fermi surfaces with itinerant f electrons and strongly enhanced effective masses. How and where the FSs and effective masses change as a function of Ir concentration is one of the important open questions, which we addressed within

### Visiting Scholars

this project. To this end, high quality single crystals of CeRh<sub>1-x</sub>Ir<sub>x</sub>In<sub>5</sub> with several different concentrations of Ir were grown. Figure 1(b) shows the Fourier spectra of the dHvA oscillations in CeRh<sub>0.8</sub>Ir<sub>0.2</sub>In<sub>5</sub> and CeRh<sub>0.4</sub>Ir<sub>0.6</sub>. For both compositions, the observed dHvA frequencies and effective masses are the same as in pure CeRhIn<sub>5</sub>. This suggests that the FSs and effective masses in CeRh<sub>1-x</sub>Ir<sub>x</sub>In<sub>5</sub> do not change up to at least the critical concentration of Ir. This conclusion should, however, be treated with caution, as a more recent microprobe analysis revealed a significant difference between the real and nominal Ir concentrations in some of the samples. Therefore, new samples of CeRh1-xIrxIn5 are being grown. All the new crystals will be tested by microprobe and specific heat measurements, prior to dHvA studies, which will be performed, if necessary, also in high magnetic fields up to 36 T in Grenoble.

In pure CeRhIn<sub>5</sub>, the analysis of our previous dHvA results in magnetic fields up to 70 T revealed that several dHvA frequencies gradually emerge at high fields as a result of magnetic breakdown. Among them is the thermodynamically important  $\beta_1$ branch, which has not been observed so far. Comparison of our angular-dependent dHvA spectra with those of the non-4f compound LaRhIn<sub>5</sub> and with band-structure calculations evidences that the Ce 4f electrons in CeRhIn<sub>5</sub> remain localized over the whole field range. This rules out any FS reconstruction, either at the suggested nematic phase transition at  $B^*$  $\approx 30$  T or at the putative quantum critical point at  $B_{\rm c}$  $\approx$  50 T. Our results rather demonstrate the robustness of the FS and the localized nature of the 4f electrons in- and outside of the antiferromagnetic phase. A manuscript based on these findings was recently submitted to Physical Review Letters.

In non-magnetic CeCoIn<sub>5</sub> and CeIrIn<sub>5</sub>, a QCP can be induced by doping, e.g. by Cd substitution into In sites. Introduction of Cd into CeCoIn<sub>5</sub> creates initially a two phase region above nominal x = 0.075, where  $T_N > T_c$ , followed by only antiferromagnetism for x >0.12. The phase diagram of CeIr(In<sub>1-x</sub>Cd<sub>x</sub>)<sub>5</sub> seems to be strikingly different. Only superconductivity was observed for  $x \le 0.025$ , while only a magnetic ground state was observed for  $x \ge 0.075$ . This ambiguity motivated us to re-examine the low-temperature properties of CeIrIn<sub>5</sub> doped with 5% of Cd, CeIr(In<sub>0.95</sub>Cd<sub>0.05</sub>)<sub>5</sub>.



Fig. 2 Superconducting transition in CeIr(In<sub>0.95</sub>Cd<sub>0.05</sub>)5 observed in specific heat (left axis) and resistivity (right axis).

As shown in Fig. 2, we observed a superconducting transition both in resistivity and specific heat. Similar to pure CeIrIn<sub>5</sub>, the transition temperature in resistivity is much higher than that determined from specific heat measurements. On the other hand, we have not observed any signature of an AFM transition. These results allowed us to revise the previously suggested temperature-concentration phase diagram of CeIr(In<sub>1-x</sub>Cd<sub>x</sub>)<sub>5</sub>. Furthermore, we have confirmed beyond any doubt that superconductivity does not co-exist with antiferromagnetism in Cd-doped CeIrIn<sub>5</sub>. An article based on these results together with those of our previous neutron diffraction study of CeIr(In<sub>0.9</sub>Cd<sub>0.1</sub>)<sub>5</sub> was recently published in Physical Review B [1].

Finally, several new samples of the recently discovered spin-triplet superconductor  $UTe_2$  were grown and tested. This allowed us to further master the growing technique of this fascinating material. Consequently, high quality single crystals of  $UTe_2$  were grown in the CEA-Grenoble. One of these crystals was chosen for the future dHvA experiments in high magnetic fields.

#### **References**

[1] K. Beauvois, N. Qureshi, R. Tsunoda, Y. Hirose, R. Settai, D. Aoki, P. Rodière, A. McCollam, and I. Sheikin, Phys. Rev. B 101, 195146 (2020).

[2] L. Llobet et al., Phys. Rev. Lett. 95, 217002 (2005).

Keywords: heavy fermion, Fermi surface, electronic structure Dr. Ilya Sheikin (LNCMI-Grenoble, CNRS, Grenoble, France) E-mail: ilya.sheikin@lncmi.cnrs.fr

#### Domain structure and current induced switching in synthetic antiferromagnetic thin films of CoGd

Synthetic antiferromagnetic multilayers of CoGd with opposite net magnetic moment are grown and investigated by means of Kerr microscopy. The composition is optimized for compensation to be near the room temperature for optimal spin-orbit-torque switching in patterned structures. The effect of charge current pulses on magnetization processes is observed.

Antiferromagnets (AF), possessing relatively small susceptibility and demonstrating no stray fields are possible candidates for breakthrough on the memory density with no inter-bit influence [1]. However, direct write and read in true antiferromagnets are associated with certain difficulties. Synthetic antiferromagnetic, composed of ferrimagnetic layers with opposite net magnetic moments are more suitable for such memory applications.

Recently, spin orbit torque was shown to be applicable for switching of magnetic state in bilayers of CoGd [2,3]. Two layers of CoGd with different compositions (Co-rich and Gd-rich) grown between thin Pt layers were patterned in cross bars and charge current was passed through. Most of the current flows within the Pt layer and generates a spin torque on CoGd bilayer from top and bottom side, large enough to switch the magnetic state of bilayers, detected as change in Hall resistance.

In our study we have prepared films with the bilayer stack repeated 2 or 3 times (Fig. 1a), which should allow for higher efficiency of spin torque. The thickness of Pt layer was always 2 nm and thickness of independent CoGd layers was from 3 nm (for structures with 3 repetition) to 4 nm (for that with 2 repetition). We have optimized the composition of CoGd layers to have compensated films near the room temperature and patterned films in a shape of wires to apply current pulses (Fig. 1b). Magnetic observed by domains were means of magneto-optical Kerr microscopy with opportunity for selective sensitivity [4], determined by polarized light incidence (Fig. 1 d,e). All-directional field application within the sample plane was realized with help of quadrupole coil (Fig. 1 c).

This report presents results on a film with compensation temperature at around 305 K. Fig. 2a demonstrates typical domain structure, observed in zero field after demagnetization in AC field (Kerr sensitivity is shown by red arrow). Optically measured magnetization loop along the wires direction in absence of charge current is presented in Fig. 2b (black curve).

To investigate the influence of the presence of spin orbit torque effect from charge current in Pt and possibility for field-free switching of the magnetization we have applied to the patterned chip the charge current pulses at constant repetition rate of 100 Hz, varying the duration of the pulse (in percent of duty cycle) and its amplitude. Typical pulse profile can be seen in the inset to Fig. 2d: black curve is voltage applied to structure and red curve is actual current passed through. Pulse width was varied from 2  $\mu$ s to 50  $\mu$ s.



Fig. 1 (a) Layer stacks; (b) patterned bar (c) experimental setup for Kerr observations; (d, e) Sensitivity principle in Kerr microscopy

The Fig. 2b demonstrates the influence of current passing through the structure with DC current (red curve) and pulsed current (blue and green curves). Although we observe no bias effect, the reduction in coercivity can be clearly seen. By varying the amplitude of the current pulse and its duration, we obtained the dependence of the coercivity on current amplitude, represented in Fig. 2c. The correspondent current density is shown at the top scale of the plot and absolute values are critical current, closed to required for magnetization switching, reported in [2].

However, the reduction in coercivity could also be associated with increase of sample temperature due to resistive heating (the total

### Visiting Scholars

resistance of the chip is around 500 Ohm). To evaluate such an opportunity, a series of experiments with pulses of the same amplitude, but different pulse duration and thus different heat per pulse have been performed. As it can be seen from Fig. 2d for the pulses with drastically diverse heat per pulse the coercivity values are not so divergent if the pulse amplitude is kept at the same level, while as a function of current amplitude Hc demonstrates a clear linear trend. This allows to conclude that the reduction in coercive field is associated rather with effect of charge current passing the wires and exciting the magnetization oscillations at domain boundaries.

The resistivity of Pt is usually orders of smaller than that of CoGd, thus the current mostly flows through the Pt layer, what creates additional Oersted field in adjacent CoGd layer. This field is, however, compensated by field of opposite sign generated by Pt layer from other side of CoGd layer. Oersted field emerging from neighbouring wires the is completely compensated for the wire in a middle of the structure as it comes from symmetry reasons (in total we have 5 wires at 20 µm distance from each other) and as we observe no difference in behaviour between the middle wire and wire on a

side we may deduct, that the influence of Oersted field on side wires can be also neglected.

The direct effect from charge current pulses on domain structure can be unequivocally seen if pulses are applied in absence of the external field. For that purpose a certain domain pattern was prepared (Fig. 2a) and saved as a reference image. Then a pulse train was sent through the chip and by subtracting the reference image with original domains from live image we can observe only the change in domain structure (Fig. 2 e and f).

These findings allow the deduction that the grown multilayers of CoGd/Pt demonstrate the possibility for current induced switching and can be investigated by means of Kerr microscopy. Further study is in progress.

#### <u>References</u>

 A. Manchon, I. M. Miron, T. Jungwirth, J. Sinova, J. Zelezny, A. Thiaville, K. Garello and P. Gambardella, Rev. Mod. Phys. 91, 035004 (2019)

[2] T. Moriyama, W. Zhou, T. Seki, K. Takanashi and T. Ono, Phys. Rev. Lett. **121**, 167202 (2018)

[3] W. Zhou, T. Seki, T. Kubota, G. E. W. Bauer and K. Takanashi, Phys. Rev. Mat. **2**, 094404 (2018)

[4] I.V. Soldatov, R. Schafer, Rev. Sci. Instrum. **88**, 073701 (2017)



Fig. 2 (a) typical domain structure in demagnetized state; (b) magnetization loops measured along the wire; (c and d) coercive field as a function of current pulse amplitude and Joule heat in pulse; (e and f) change in domain structure after current pulse observed in longitudinal and transversal sensitivities (shown as red arrows).

Keywords: spin current, magnetic properties, magnetooptic

Ivan Soldatov (Leibniz Institute for Solid State and Materials Research, Dresden, Germany) E-mail: i.soldatov@ifw-dresden.de

https://www.ifw-dresden.de/magnetics#c8043

# Investigations on the mechanical behavior of 3D interconnected composites developed by liquid metal dealloying

wo challenging ideas were proposed to improve the mechanical properties of 3D interconnected composites produced by liquid metal dealloying. The two approaches were based on the enhanced interface bonding via elaborate alloying design and severe plastic deformation. Firstly, an additional Ni or Al in the Mg melt can act as "glue" on the immiscible interface between FeCr ligaments and the Mg melt phase. Consequently, the work-hardening induced excellent ductility was achieved as stress-drop and restoration signals in the tensile stress-strain curve. Secondly, the high-pressure torsion process leads to structural diversification into the nanolayered structure, probably with improved interface bonding by atomic shuffling.

Metal matrix composites, MMCs, are a material with at least two constituent phases, one corresponds to a metal matrix as a continuous phase, and the other phase should be a different metal or another material such as a ceramic or organic compound. The later phase provides a better level of physical properties such as high strength, high stiffness, or lighter weight to the composite. Conventionally, MMCs are classified on the basis of reinforcing phases depending on their shapes.

Properties of these MMCs are judged by not only each phase's properties itself, but also by several factors such as shape, fraction, size, uniformity of distribution, interface bonding, etc. However, the property changes, which brought by the additional second phase, are highly influenced by the fraction of reinforcements in general. Therefore, the simple rule-of-mixture equation is often used to estimate the properties of MMCs. This tendency indicates that it is hard to overcome the trade-off phenomenon between the two properties. Even some times, some composite materials show a negative hybrid effect.

The visiting professor (Prof. H.S. Kim) and the host professor (Prof. Kato) suggested the new types of composites, which are based on 3D interconnected structure, to obtain a strong positive hybrid effect. Liquid metal dealloving (LMD) is a newly discovered technique in 2011 by the group of Prof. Kato, and this dealloying method can develop individually 3D interconnected two phases by utilizing a molten metal as a dealloying medium [1-6]. Two phases form a continuously disordered structure, and it leads to a large interface area by constructing an interlocked morphology. The size of the features is from nanometer to a few micron scales, which providing much smaller levels compared to those of conventional MMC materials. The interlocked construction can enhance the strength of composite as well as ductility. The interface acts as an efficient barrier against dislocation motion, and this complex geometric structure provides hydrostatic pressure for the brittle phase during deformation. Thus, the crack propagation can be prevented.

However, 3D interconnected composite developed by a simple LMD triangle has an immiscible character of the interface. Therefore, the interface bonding should be weak. Without good interface strength, strong positive hybrid effects would not be expected. To overcome this undesirable phenomenon, the visiting professor and the host professor started pioneering investigations with two approaches; 1) elaborate alloying design & 2) atomic shuffling via severe plastic deformation.



Fig. 1. (a) Modified triangle relationship of the enthalpies of mixing via the elaborated alloying design of the melt. (b) FeCr/Mg composite with additional Ni in the melt. (c) Tensile stress-strain curves of FeCr/Mg composites produced by the LMD process. (d) Fracture surface of the composite with Al.

The first idea is based on carefully designed LMD systems with minor alloying elements in the metallic melt (Fig. 1a). The previous invention considered only a pure metallic melt and the simple miscibility relationships among the precursor elements and the metallic melt element for the selective dissolution of a miscible component. Two different minor alloying elements were selected to study the role of its chemical affinities with precursor elements and the metallic melt element. In the simple LMD

### Visiting Scholars

system of (Fe<sub>80</sub>Cr<sub>20</sub>)<sub>50</sub>Ni<sub>50</sub> precursor and Mg melt, 4 at.% of Ni or Al was added in the Mg melt. The minor alloying element of Ni resulted in the eutectic structure of Mg and Mg<sub>2</sub>Ni intermetallic. The high concentration of Ni in the melt also led to the enhanced interface bonding between FeCr ligaments and those melt phases (Fig. 1b).

Mg composite with Mg<sub>2</sub>Ni intermetallic has been known as extremely brittle. However, in the complex geometry of the LMD composite, the fracture of Mg<sub>2</sub>Ni, as well as Mg, can be delayed. Furthermore, enhanced bonding strength prevents crack propagation through the 3D interlocked morphology. Consequently, the work-hardening induced excellent ductility could be achieved as stress-drop and restoration signals in the stress-strain curve (Fig. 1c).

The minor alloying element of Al also demonstrated the improved interface bonding on the fracture surface. Pure Mg melt sample clearly showed the distinct debonding behavior during the tensile loading, and it exhibited limited elongation. Near the interface, ligaments and melt phase depicted different levels of plastic deformation. On the other hand, most of the interface area was tightly bonded in the AI added sample even after a fracture (Fig. 1d). Al is miscible to both ligament elements (Fe and Cr) and Mg melt. The added 4.0 at.% of Al did not produce the second phase, but it produced a solid solution phase with Mg. Furthermore, the high chemical affinities of Al with Fe and Cr cause the bulk diffusion of AI atoms into the ligament, and they might act as "glue" at the immiscible FeCr-Mg interface.



Fig. 2. (a) 3D microstructure of the LMD composite and schematic diagram of shear strain by HPT process. (b) Interlocked nanolayers after the HPT process.

Keywords: composite, 3d structure, mechanical properties Hidemi Kato (Non-Equilibrium Materials Research Laboratory) E-mail: hikato@imr.tohoku.ac.jp URL: <u>http://www.nem2.imr.tohoku.ac.jp/index-e.html</u>

Hyoung Seop Kim (Pohang University of Science and Technology) Email: hskim@postech.ac.kr

Severe plastic deformation was the second idea. The high-pressure torsion (HPT) process can apply shear strain over ~100 under high hydrostatic pressure without fracture (Fig. 2a). The disordered interlocked composite structure of LMD was diversified into the nanolayered structure (Fig. 2b). Not only the structural changes and grain refinement, but also it would be useful to improve interface strength through atomic shuffling via severe deformation. Thus, the HPT processed LMD composite would result in high strength and good ductility. Furthermore, the limited path along the vertical direction of the interlocked nanolayers has a high potential to develop new nanocomposite materials for diffusion or thermal barriers.

#### <u>References</u>

[1] T. Wada, K. Yubuta, A. Inoue, and H. Kato, Mater. Lett. **65**, 1076 (2011).

[2] T. Wada, P.-A. Geslin, H. Kato, Scr. Mater. **142**, 101 (2018).

[3] S.-H. Joo, T. Wada, and H. Kato, Mater. Des. **180**, 107980 (2019).

[4] S.-H. Joo, K. Yubuta, and H. Kato, Scr. Mater. **177**, 38 (2020).

[5] S.-H. Joo, and H. Kato, Mater. Des. 185, 108271 (2020).

[6] S.-H. Joo, J.W. Bae, W.-Y. Park, Y. Shimada, T. Wada, H.S. Kim, A. Takeuchi, T.J. Konno, H. Kato, I.V. Okulov, Adv. Mater. 32, 1906160 (2020).

2

# **Activity Report**

Workshops

# Workshops

Term	2019.9.17-21	2019.10.29-30	2019.2.10-11	2019.11.27-28
Place	Kobe University	KIST, Korea	Sendai International Center	IMR Auditorium
Title of Workshop	J-Physics 2019 International Conference & KINKEN-WAKATE 2019 Multipole Physics	KINKEN-KIST Joint Workshop 2019	The 3rd Symposium for The Core Research Clusters for Materials Science and Spintronics	Summit of Materials Science 2019 and GIMRT User Meeting 2019
Chairperson or Committee Member	Prof. Aoki	Prof. Sasaki	Prof. Sasaki	Prof. Takanashi
Application No.	19WS01	19WS02	19WS03	19WS04

# Workshops

### J-Physics 2019 International Conference & KINKEN-WAKATE 2019 Multipole Physics

We organized the international workshop "KINKEN-WAKATE 2019 Multipole Physics" at Centennial Hall in Kobe University, as a joint workshop with J-Physics 2019 International conference from Sep 17 to Sep 21, 2019. Many researchers and students participated in this joint workshop, leading to fruitful discussion, future international collaboration, and encouragement for young researchers.

The purpose of this joint workshop with J-Physics2019 is the exchange and discussion on the recent experimental and theoretical achievements related to the multipole physics. The topics includes multipole order, quantum phase transition and criticality, unconventional superconductivity, parity mixing and the novel quantum phenomena, dynamical response by augmented multipole, development of new materials based on the strong spin-orbit coupling. In the first two days, KINKEN-WAKATE 2019 was held as a tutorial session, where 5 distinguished lecturers gave their lectures mainly for young researchers and students. topics The covers spin-triplet superconductivity, topological insulator/ superconductor, augmented multipole, high field experiment, Ab initio calculation. We also had short oral presentations by students who have their posters. After KINKEN-WAKATE 2019, we had J-Physics 2019 international conference, where 34 invited talks, 14 contributed talks were given for four days. The sessions consisted of several topics related to multipole physics, namely "EuPtSi, Skyrmion, Yb-system", "1-2-20 system", "Solid state chemistry and new materials", multipole", "Magnetic "Augmented multipole", "Novel superconductor UTe2", "Exotic superconductivity" and topics". "Miscellaneous interesting The details are shown in the following program. In poster sessions, we had 92 poster presentations for two days. To encourage young researchers, 8 posters were selected as "Best Poster Awards". There were 155 participants including 18 from abroad, France, Germany, The Netherlands, USA, China, Korea, Croatia. The proceedings of J-Physics 2019 has been published in JPS Conference Proceedings Vol.29 in 2020.

I would like thank all participants, local staffs, members of local committee, program committee, publication committee on behalf of the organizing committee. I acknowledge also the financial support and suggestions by ICC-IMR.



Fig. 1 Photograph of J-Physics 2019 International Conference & KINKEN-WAKATE 2019 Multipole Physics

Keywords: multipole, magnetism, superconductivity Dai Aoki (Actinide materials science group) E-mail: aoki@imr.tohoku.ac.jp http://actinide.imr.thoku.ac.jp/

### Workshops

Table I: Program for "KINKEN-WAKATE 2019 Multipole Physics" and "J-Physics 2019"



J-Physics 2019 International Conference & KINKEN-WAKATE 2019 Multipole Physics KINKEN-WAKATE 2019 Tutorial Session : Sep. 17, 13:00 – Sep. 18, 11:15 J-Physics 2019 International Conference : Sep. 18, 13:00 – Sep. 21, 12:30

Centennial Hall (Rokko Hall), Kobe University (Rokkodai 1-1, Nada-ku, Kobe 657-8501 Japan)



Sep 17 (Tue)

#### **KINKEN-WAKATE** Opening

13:00 - 13:05	Opening remarks		
<b>Tutorial Sessio</b>	n		
13:05 - 14:05	Jean-Pascal Brison Univ. Grenoble Alpes, CEA, Pheliqs	p-wave superconductivity in uranium based systems	
14:15 - 15:15	Anne de Visser <i>University of Amsterdam</i>	Topological insulators and superconductors	
15:25 - 16:25	Satoru Hayami Hokkaido University	Augmented multipoles and cross-correlated couplings	
Sep 18 (Wed)			
9:00 - 10:00	Ilya Sheikin LNCMI, CNRS	Experimental techniques in high magnetic field	

Harald O. Jeschke	Ab initio calculations for strongly correlated electron systems

#### J-Physics 2019 Opening

10:15 - 11:15

13:00 - 13:10		Opening remarks
EuPtSi, Skyrmie	on, Yb-system	
13:10 - 13:40	Catherine Pappas Delft University of Technology	Novel low temperature spiral and skyrmionic states
13:40 - 14:00	Yoshichika Onuki <i>University of the Ryukyus</i>	Single crystal growth and unique electronic states of cubic chiral EuPtSi and related compounds
14:00 - 14:20	Koji Kaneko Japan Atomic Energy Agency	Skyrmion lattice in f-electron magnet EuPtSi: neutron scattering study
14:20 - 14:40	Chihiro Tabata <i>Kyoto University</i>	Resonant X-ray scattering study of magnetic order in chiral antiferromagnet EuPtSi
14:40 - 14:55	Shigeo Ohara Nagoya Institute of Technology	$\begin{array}{llllllllllllllllllllllllllllllllllll$
14:55 - 15:15	Takeshi Matsumura <i>Hiroshima University</i>	Chiral soliton lattice formation in Yb(Ni <sub>1-x</sub> Cu <sub>x</sub> ) <sub>3</sub> Al <sub>9</sub>

#### 1-2-20 System

15:45 - 16:15	Sung Bin Lee KAIST	Field effect of multipolar order and superconductivity
16:15 - 16:45	Atsushi Tsuruta <i>Osaka Univ.</i>	Non-Fermi liquid behaviors in two-channel Anderson impurities and lattice model
16:45 - 17:05	Yu Yamane <i>Hiroshima University</i>	Non-fermi liquid behaviors in diluted $4f^2$ systems $Y(Pr)T_2Zn_{20}$ $(T=Ir \mbox{ and }Co)$
17:05 - 17:25	Tatsuya Yanagisawa <i>Hokkaido University</i>	Logarithmic elastic response in the dilute non-Kramers system $Y_{1\text{-}x}Pr_xIr_2Zn_{20}$

Sep 19 (Thu)

#### Solid State Chemistry and New Materials

9:00 - 9:30	Yanpeng Qi School of Physical Science and	Pressure-induced superconductivity and topological quantum phase transitions in topological materials
	Technology,ShanghaiTech University	
9:30 - 9:50	Yoshihiko Okamoto <i>Nagoya University</i>	Superconductivity in PtSbS with noncentrosymmetric and cubic crystal structure
9:50 - 10:10	Hiroyuki Yoshida <i>Hokkaido University</i>	Application of hydrothermal technique to develop 3d transition metal compounds without local inversion symmetry
10:10 - 10:25	Kosmas Prassides <i>Osaka Prefecture University</i>	Emergent electronic phenomena in hybrid f-/p-electron molecular materials

#### Augmented Multipole I

10:55 - 11:15	Satoru Hayami <i>Hokkaido University</i>	Momentum-dependent spin splitting by collinear antiferromagnets without atomic spin-orbit coupling
11:15 - 11:35	Tomoya Higo ISSP, University of Tokyo	Large spontaneous responses induced by ferroic order of cluster magnetic octupoles in $Mn_3Sn$
11:35 – 11:55	Yuki Yanagi Institute for Materials Research, Tohoku University	Spontaneous inversion symmetry breaking by electric toroidal quadrupole ordering in $Cd_2Re_2O_7$
11:55 - 12:10	Masashi Takigawa ISSP, University of Tokyo	Noncentrosymmetric phases in the spin-orbit coupled metal $Cd_2Re_2O_7$ : Cd-NMR
12:10 - 12:25	Changle Liu Fudan University	Detecting hidden order in frustrated magnets

#### **Miscellaneous Interesting Topics**

13:30 - 14:00	Toni Helm Helmholtz-Zentrum Dresden- Rossendorf	Pulsed magnetic field, high pressure and FIB microstructures - a powerful combination for studies of unconventional metals
14:00 - 14:30	Yejun Feng Okinawa Institute of Science and Technology Graduate University	Direct observation of continuous all-in-all-out quantum phase transition under pressure
14:30 - 14:50	Noriaki Kimura <i>Tohoku University</i>	Orbital crossing and magnetic breakdown in noncentrosymmetric metals
14:50 - 15:10	Ryuji Higashinaka Tokyo Metropolitan University	Unconventional strongly correlated electronic states induced by multiple degrees of freedom in cubic Sm compounds
15:10 - 15:25	Ryousuke Shiina University of Ryukyus	Theory of valence fluctuation and magnetic ordering in nearly trivalent Eu compounds

Sep 20 (Fri)

UIe <sub>2</sub>
------------------

9:00 - 9:30	Sheng Ran University of Maryland & NIST	Unusual superconducting state in nearly ferromagnetic compound $UTe_2$
9:30 - 10:00	Georg Knebel Univ. Grenoble Alpes and CEA Grenoble	Field enhancement of superconductivity close to the metamagnetic transition in $UTe_2$
10:00 - 10:20	Kenji Ishida <i>Kyoto University</i>	NMR studies on U-based superconductors
UTe <sub>2</sub> II		

10:50 – 11:10	Atsushi Miyake ISSP, The University of Tokyo	Meta	magneti	sm in heavy ferm	ion superconduct	ors UTe	2
11:10 - 11:25	Daniel Braithwaite Univ. Grenoble Alpes and CEA Grenoble	The press	nearly ure	ferromagnetic	superconductor	$UTe_2$	under

#### 3

## Workshops

11:25 - 11:40	William Knafo LNCMI/CNRS, Toulouse, France	Investigation of metamagnetism and reentrant superconductivity in $UTe_2$ by resistivity under intense pulsed magnetic field
11:40 - 11:55	Jun Ishizuka <i>Kyoto University</i>	Insulator-metal transition and odd-parity topological superconductivity in $UTe_2$
11:55 - 12:10	Suguru Hosoi <i>Osaka University</i>	Thermal conductivity measurements of the $UTe_2 \\ superconductor$

#### Exotic Superconductivity I

13:10 - 13:40	Clifford W. Hicks Max Planck Institute for	An evaluation of chiral superconductivity in Sr <sub>2</sub> RuO <sub>4</sub>
	Chemical Physics of Solids	
13:40 - 14:05	Shunichiro Kittaka ISSP, University of Tokyo	Thermodynamic study of the superconducting gap structure of $\mathrm{Sr}_2\mathrm{RuO}_4$
14:05 - 14:30	Shingo Yonezawa Graduate School of Science, Kyoto University	Probing and tuning of nematic superconductivity in doped $Bi_2Se_3$ superconductors

#### Augmented Multipole II

14:40 - 15:10	Di Xiao <i>Carnegie Mellon University</i>	Theory of magnetoelectric multipoles and its application in transport and optical effects
15:10 - 15:30	Motoi Kimata Institute for Materials Research, Tohoku University	Magnetic spin Hall effects in a non-colinear antiferromagnet
15:30 - 15:45	Shinji Watanabe <i>Kyushu Institute of Technology</i>	Charge transfer effect under odd-parity crystalline electric field: divergence of magnetic toroidal fluctuation in $\beta$ -YbAlB <sub>4</sub>

#### Sep 21 (Sat)

#### **Magnetic Multipoles**

9:00 - 9:20	Gaku Motoyama Shimane University	Magnetoelectric effect in antiferromagnetic ordered state of $Ce_3TiBi_5$ with Ce zig-zag chains
9:20 - 9:40	Akinari Koriki <i>Hokkaido University</i>	Observation of magnetoelectric effect in antiferromagnetic metal $CeRu_2Al_{10}$
9:40 - 10:00	Yuki Shiomi University of Tokyo	Observation of a magnetopiezoelectric effect in the antiferromagnetic metal $EuMnBi_2$
10:00 - 10:20	Kenya Ohgushi <i>Tohoku University</i>	Ferroic order of magnetic quadrupoles in BaMn <sub>2</sub> As <sub>2</sub>
10:20 - 10:40	Hikaru Watanabe Department of Physics, Kyoto University	Classification of multipole order: candidates and application to emergent responses

#### Exotic Superconductivity II and More

11:10 - 11:25	Shintaro Hoshino <i>Saitama University</i>	Unconventional full-gap superconductivity in Kondo lattice with semi-metallic conduction bands
11:25 - 11:40	Kazumasa Miyake Osaka Universtiy, Center for Advanced	Spin-orbit-phonon interaction as an origin of helical-symmetry breaking spin-triplet superconducting state
	High Magnetic Field Science	
11:40 - 12:00	Alix McCollam <i>HFML-EMFL, Nijmegen</i>	Quantum oscillation studies of heavy fermion superconductors in high magnetic fields
12:00 - 12:20	Hilbert v. Löhneysen Karlsruhe Institute of Technology	Unusual two-band proximity-induced superconductivity in a simple metal: contribution of bulk and surface states in silver islands on (110)-oriented niobium

#### KIST-KINKEN Joint Workshop 2019

Korea Institute of Science and Technology (KIST) is a long-term partner institute of IMR and Tohoku University. Alternating "KINKEN-KIST joint symposium" in Sendai and Seoul are important for connecting each researches by exchanging the idea in the broad range of the materials science. Among several research institutes in KIST, Post-Silicon Semiconductor Institute (PSI) is a Key institute for materials science. In 2019, "PSI (Post-Silicon Semiconductor Institute) – KINKEN Joint Workshop 2019" was held at KIST

"KINKEN - KIST Joint Workshop 2019" was held at a lecture hall in International Cooperation Building, Korea Institute of Science and Technology (KIST), Seoul, on 29-30 October 2019. Tohoku University has a long history of academic exchange with KIST. As a commemoration of concluding university - level academic exchange agreement between KIST and Tohoku University in 2016, Institute for Materials



Fig. 1 Opening remarks by Director Dr. Joonyeon Chang and introduction of IMR by Director Prof. Koki Takanashi

Research (IMR, KINKEN) and KIST jointly held a "KINKEN-KIST joint seminar" in Sendai, and that led to a series symposium in 2017 in Seoul and in 2018 in Sendai alternatively. In 2019, director of IMR, Prof. Koki Takanashi and seven researches of IMR participated in this Joint Workshop by supporting from ICC-IMR.

Starting from an opening address and brief introduction of exchange history between KIST and IMR by Dr. J. Chang, director of PSI, Prof. Koki Takanashi, director of IMR, introduced recent research activities in IMR. In the scientific sessions, wide range of research topics such as spintronics, condensed matter physics and electronic materials and device applications were presented by both KIST and IMR researches. During coffee breaks, lunch and banquet time, very vigorous discussions on each presentation and future plan for effective exchange between PSI/KIST and IMR were conducted. In the morning of the second day, lab tours in KIST and group discussions were carried out.

We will deepen an academic relationship, exchange and collaboration with KIST continuously through holding this series symposium. Next symposium will be opened at IMR in 2020.



Fig. 2 Group photo at KIST in Seoul

Keywords: spintronics, electronic material, devices Takahiko Sasaki (Low Temperature Condensed State Physics) E-mail: takahiko@imr.tohoku.ac.jp

## Workshops

#### Program

□ Oct. 29(Tues.)	
08:50-09:00	Registration
09:00-09:15	Opening remarks, Joonyeon Chang(PSI, KIST)
09:15-09:30	Introduction of KINKEN, Koki Takanashi (IMR)

#### Session 1. Spintronics

Session Chair : Dr.	Byoung-Chul Min (Center for Spintronics, KIST)
09:30-09:55	"Electronic state and phase stability of half-metallic ferromagnets
	in Heusler alloys" Rie Umetsu (Cooperative Research and
	Development Center for Advanced Materials,IMR)
09:55-10:20	"Asymmetric motions of magnetic domain wall and skyrmion with
	the Dzyaloshinskii-Moriya interaction"
	Kyoung-Whan Kim (Center for Spintronics, PSI, KIST)
10:20-10:30	Break
10:30-10:55	"Anomalous Nernst effect in nanostructured materials",
	Masaki Mizuguch (Collaborative Research Center on Energy
	Materials, IMR)
10:55-11:20	"Chiral interlayer exchange coupling in synthetic
	antiferromagnets",
	Dong-Soo Han (Center for Spintronics, PSI, KIST)
11:20-11:45	"Spin-charge conversion in ferromagnetic materials"
	Takeshi Seki (IMR)
11:45-12:10	"Charge density wave order in 2D transition metal
	dichalcogenides"
	Hyejin Ryu (Center for Spintronics, PSI, KIST)
12:10-13:10	Lunch (Group Photo)

#### Session 2. Electronic materials

Session Chair : Dr.	Chong-Yun Kang (Center for Electronic Materials, KIST)
13:10-13:35	"Epitaxial Piezoelectric Thin Films on Si for Ultrasound Transducers",
	Seung-Hyub Baek (Center for Electronic Materials, PSI, KIST)
13:35-14:00	"Magnetroelectric effects in the quantum spin dimer system",
	Shojiro Kimura(High field laboratory for Superconducting Materials,

	IMR)
14:00-14:25	"Trap analysis and IR applications of colloidal quantum dots",
	Gyu Weon Hwang (Center for Electronic Materials, PSI, KIST)
14:25-14:50	"New aspects of Sn-based transparent conducting oxides:
	high-mobility interface and its potential coupling with spontaneous
	polarization" Kohei Fujiwara (IMR)
14:50-15:15	"Stress-Composition Coupling in Li Alloys and Their Applications"
	Sangtae Kim (Center for Electronic Materials, PSI, KIST)
15:15-15:30	Break

Session 3. Devices and Semiconductor Materials

Session Chair : Dr. Jin-Dong Song(Center for Opto-Electronic Materials and Devices,

PSI, KIST)

. ,	
15:30-15:55	"π-electron physics in organic molecular materials,
	Takahiko Sasaki (IMR)
15:55-16:20	"Heterogeneous optical phase modulation for Si photonics"
	Jae-Hoon Han (Center for Opto-Electronic Materials and Devices,
	PSI, KIST)
16:20-16:45	"Neutron-Scattering Study of Electron-Doped High-Tc Cuprate
	superconductor"
	Masaki Fujita (IMR)
16:45-17:00	"Introduction to CMOS-Compatible Single-Photon Avalanche
	Diodes And Their Applications",
	Myung-Jae Lee(Center for Opto-Electronic Materials and Devices
	Research, PSI, KIST)
17:00-17:30	Closing remarks
	Koki Takanashi (IMR) / Joonyeon Chang(PSI, KIST)

□ Oct. 30(Wed.)

10:00-11:30 Lab. tour (MBE)

### Workshops

#### The 3rd Symposium for The Core Research Clusters for Materials Science and Spintronics

he 3rd Symposium for The Core Research Clusters for Materials Science and Spintronics was held at Sendai International Center (Sendai, Japan) from February 9<sup>th</sup> to 11<sup>th</sup> 2020. The symposium consisted of 3 plenary speeches and 10 sessions which included 30 presentations and 86 poster presentations. About 250 researchers from all over the world participated this symposium, and we could show our research results and discuss future prospects.

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, Tohoku University initiated the Core Research Clusters in four research fields; materials science, spintronics, next-generation medical care and disaster science. We held the 3rd symposium on the two research fields, Materials Science and Spintronics at Sendai International Center (Sendai, Japan) from February 9th to 11th 2020 to show our research results and discuss future prospects.



Fig.1 Opening Remarks by Prof. Hideo OHNO, President of Tohoku University



Fig.2 Prof. Yoshiro HIRAYAMA, Director of Core Research Cluster for Spintronics. Chair of Plenary session.

Totally 3 Plenary speakers, 23 invited speakers, about 250 participants from 10 countries, and 86 poster presenters joined the symposium. The details are as follows;

#### (1) Plenary Session

The first plenary speaker, Prof. Jerome B. HASTINGS, from SLAC National Accelerator Laboratory, USA, provided a lecture titled "Challenges and Opportunities with SLIT-J". The second plenary speaker, Prof. Stéphane MANGIN, from University of Lorraine, France, gave a lecture titled "Single femto second ferromagnetic to switch layers laser mediated by spin transport". The last plenary speaker, Prof. Maki KAWAI, who is Director General, Institute for Molecular Science, Japan, spoke on "Cutting edge research to lead materials science"



Fig.3 Plenary speakers; Prof. Jerome B. HASTINGS, Prof. Stéphane MANGIN, Prof. Maki KAWAI, from the photo left.

#### (2) Sessions for Materials

The topic of the 1<sup>st</sup> session was on High Strength Materials chaired by Prof. Kyosuke YOSHIMI. The 2<sup>nd</sup> session was on the Biomaterials chaired by Prof. Ayumi HIRANO-IWATA. The 3<sup>rd</sup> session was on Advanced Electronic Materials chaired by Prof. Tomoteru FUKUMURA. The 4<sup>th</sup> session was on Advanced Energy Materials Chaired by Prof. Shin-ichi ORIMO. And the last session was on Materials Development Based on Microstructure Control chaired by Prof. Tadashi FURUHARA.

1



Fig.4 Lectures from invited speakers

#### (3) Sessions for Spintronics

The topic of the 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> session was on the Spintronics Materials Research chaired by Prof. Koki TAKANASHI, Prof. Masafumi SHIRAI and Prof. Shigemi MIZUKAMI. The 4<sup>th</sup> session was on Spintronics Fundamental Research by Junsaku NITTA. And the last session was on Spintronics Device Research chaired by Prof. Fumihiro MATSUKURA.

#### (4) Poster Session

Committee members reviewed total 86 posters and bestowed the best poster award on 5 researchers and poster award on 3 researchers.

#### **Acknowledgements**

This symposium was held in collaboration with and partially supported by International Collaboration Center, Institute for Materials Research, Tohoku University. We take this opportunity to thank all the support and collaboration.



Fig.5 Discussions at Poster Session



Fig.6 Best Poster Award winners



Fig.7 Participants of "The 3rd Symposium for The Core Research Clusters for Materials Science and Spintronics"

## Workshops



#### The 3rd Symposium for The Core Research Clusters for Materials Science and Spintronics February 9 (Sun) - 11 (Tue), 2020 Jointly organized with AMIS 2020



CORE RESEARCH CLUSTER as of February 6 at Sendai International Center

Feb 9 (Sun)	Feb 1	0 (Mon)	Feb 1	1 (Tue)
	Regis	itration	Regis	stration
	Opening Remark	s (9:00-9:10) [Hagi]	Session 3 Parallel	(9:00-10:30) Session
	Chair: Yoshiro Hirayama Hideo Ohno, President of Tohoku U	niversity	<spintronics> [Tachibana] Chair: Shigeni Mizukami 10-A. Christina Paaroudaki (Cattech) 15-A. Yutaka Tabuchi (Ibe Univ. of Tokyo) 2-A. Kon Jichi Hchida (Ibational Institute</spintronics>	«Materials Science» [Fig]] Chair: Tconferu Fukumura 10-II. Hiroko Yamada (Nara Institute of Science and Technology) 11-II. Masataka Higanhiwaki (NICT) 12-JR. Fini Manaritari (Mathue for 12-JR. Fini Manaritari (Mathue for)
	Plenary Sessio	on (9:10-11:25) [Hagi]	for Materials Science)	Molecular Science)
	Chair: Yoshiro Hirayama		Coffee bre	ak (20 min.)
	1. Jerome B. Hastings (SLAC Natio	onal Accelerator Laboratory)	Session 4 (	10:50-12:20)
	2. Stéphane Mangin (University of I	Lorraine)	Parallel	Session
	3. Maki Kawai (Institute for Molecul	lar Science)	[Tachibana]	[Hagi]
Satellite Event Glass Workshop (Meeting Room, 1st floor, AIMR Main			Chair: Junsaku Nitta 13-A. Jian-Ping Wang (Univ. of Minnesota) 14-A. Samito Tsunegi (AIST) 15-A. Shunsuke Fukami (Tohoku Univ)	Chair: Shin-ichi Orimo 13-II. Miho Yamauchi (Kyushu Univ) 14-II. Gerri EW. Bauer (Tohoku Univ) 15-II. Hirotomo Nishihara (Tohoku Univ)
Bidg.)	Lunch & Poster Session 8 (11:25	& Free Discussion [Sakura] -13:40)	L (12:20	unch -13:20)
	Session 1 ( Parallel	13:40-15:10) Session	Session 5 ( Parallel	13:20-14:50) Session
	<spintronics:csrn> [Tachibana] Chair: Koki Takanashi 4-A. Yihong Wu (National Univ. of Singapore) S-A. Masaaki Tanaka (The Univ.of Tokyo) 6-A. Takeshi Seki (Tohoitu Univ)</spintronics:csrn>	Allaterials Science> [Hagi] Chair: Kyosuke Yoshimi 4-II. An-Chou Yeh (National Tsing Hua Univ) 5-B. Oleg Vasylkiv (National Institute for Materials Science) 6-II. Hiroyuki Yasuda (Osaka Univ)	«Spintronics:GP-Spin» [Tachibana] Chair: Fumihiro Matsokura 16-A. Joseph Barker (Univ. of Loeds) 17-A. Yusuke Nambu (Tohoku Univ) 18-A. Akira Kamimaki (Tohoku Univ) 19-A. Koichi Oyanagi (Tohoku Univ)	«Materials Science» [Hagi] Chair: Tadashi Furuhara 16.1. Wenzheng Zhang (Tsinghua Univ) 17.8. Nobuhiro Tsuji (Kyoto Univ) 18.8. Ryosuke Kainuma (Tohoku Univ) Toshihro Omori (Tohoku Univ) 19.4. Goro Miyamoto (Tohoku Univ)
	Coffee bre	ak (20 min.)	Poster Award Cer	remony (14:50-15:00)
	Session 2 ( Parallel	Session		
	«Spintronics» [Tachibana]	<materials science=""> [Hagi]</materials>	Closing Remar Motoko Kotani, Director of Core Re	ks (15:00-15:10) search Cluster for Materials Science
	Chair: Masafumi Shirai 7-A. Andrew Sachrajda (NRC Canada) 8-A. Shiro Saito (NTT) 9-A. Tomohiro Otsuka (Tohoku Univ)	Chair: Ayumi Hirano-Iwata 7-8: Yi-Tao Long (Nanjing Univ) Matsuhiko Nishizawa (Tohoku Univ) 8-8: Andreas Offenhiusser (Forschungszentrum Jülich) 9-8: Kaora Tamada (Kyusha Univ)		
Registration (16:00-)	Poster Session (17	7:00-17:30) [Sakura]	1	
	Move to Ban	iquet (60 min)	]	
Welcome Reception (17:00-19:00) [Sendai Kokusai Hotel]	Banquet (18:30-20:00)	[Sendai Kokusai Hotel]		

Fig.8 shows the program of The 3rd Symposium for The Core Research Clusters for Materials Science and Spintronic

3

#### Summit of Materials Science SMS 2019 and Global Institute for Materials Research Tohoku (GIMRT) User Meeting 2019, 27<sup>th</sup>-29<sup>th</sup> November

The Summit of Materials Science (SMS) 2019 and Global Institute for Materials Research Tohoku (GIMRT) User Meeting 2019 were jointly held in November 27<sup>th</sup>-29<sup>th</sup> as an international conference organized by and at the IMR. 20 invited/keynote speakers gave presentations during sessions on Spintronics and Electronics, Nuclear Engineering, Structural Materials, Energy Materials and Crystal Growth, Neutron and High Field, and so on. Younger researchers presented 72 poster.



It was to the fourth Summit of Materials Science conferences that started with SMS2011, held in the years of the Great East Japan Earthquake. SMS2016 celebrated the 100th anniversary of the IMR.

The plenary session with 20 invited speakers from Japan and abroad as well as selected IMR faculty members attracted a large audience including many interested guests from outside the IMR. The conference session on "Spintronics and Electronics", "Nuclear Engineering", "Structural Materials", "Energy Materials and Crystal Growth", "Quantum Beam and High Field" and ""Recent Activities in Research Divisions and Centers" reflected the actual IMR research topics. Speakers were selected to represent cutting-edge research in those fields and IMR staff members used the opportunity to advertise ongoing research activities.

In the afternoon of the first day of the conference, young researchers and students presenter their poster. More than 100 people gathered in the poster room to engage in heated discussions in front of the posters. A grand prizewinner and six merit award runners-up were selected from 67 competing abstracts.

The satellite workshop "GIMRTxISS-"Kibo" x AIRC" was held on the 29th. During the "Collaborative Research Platform on Ground and in Orbit" advanced research projects of three organizations were introduced and results on on various topics of aerospace and materials science were presented. The lively exchange of ideas helped promoting future collaborations.

Participants unanimously appreciated the spirit and scope of this SMS conference and are looking forward to the next installment.

# Workshops



Invited/Keynote speakers





(Upper) Poster presentation (Lower) Winners of the Young Scientist Poster Presentation Award



Nov. 27 (We	d.) : Day 1
9:00	Registration
	Opening Ceremony of GIMRT Chair: G. Bauer
	Welcome Address K. Takanashi (Director, IMR)
10:00-10:40	Greeting from President H. Ohno (President, Tohoku Univ.)
10.00 10.40	Greeting from MEXT T. Nishii (Director, SRID, RPB)
	Introduction of GIMRT Program T. Furuhara
	Scientific Session I : Spintronics and Electronics Chair: R. Umetsu
11:00-11:30	"Ferrimagnetic Spintronics" T. Ono (Kyoto Univ.) Keynote
11:30-12:00	"The Crystal Hall Effect and Topological Spintronics in Antiferromagnets" J. Sinova (Johannes Gutenberg Univ. Mainz) Keynote
12:00-12:20	"Electric Control of Magnetism in a Two–dimensional van der Waals Ferromagnet Cr <sub>2</sub> Ge <sub>2</sub> Te <sub>6</sub> " H. Kurebayashi (Univ. College London) Invited
12:20-12:40	"Spin Superfluidity Materials" W. Han (Peking Univ.) Invited
12:40.12:45	Technical Announcement H. Kato
	Group Photo
$12:45 \cdot 15:00$	Lunch and Poster (Lobby, IMR)
	Recent Activities in Research Divisions and Centers Chair: T. Sasaki
$15:00 \cdot 15:20$	"Collaborative Research with IMR Research Divisions and Groups" K. Fujiwara
15:20.15:40	"Introduction and Recent Activities of IRCNMS (Oarai Center)" Y. Nagai
15:40.16:00	"Recent Activities of HFLSM" H. Nojiri
	Scientific Session II : Nuclear Engineering Chair: S. Kondo
16:00-16:30	"Interactions of Hydrogen Isotopes and Radiation–induced Defects in Tungsten and its Impact on Performance as Plasma–facing Material of Fusion Reactor" Y. Hatano (Univ. of Toyama ) Keynote
16:30-16:50	"Dynamical Ag <sup>+</sup> –Intercalation with AgSnSe <sub>2</sub> Nano–precipitates in Cl–doped Polycrystalline SnSe <sub>2</sub> toward Ultra–high Thermoelectric Performance" L. Miao (Guilin Univ. Electronic Technology) Invited
16:50.17:10	"Metamagnetism and Superconductivity in UTe <sub>2</sub> under Intense Magnetic Field" W. Knafo (LNCMI–Toulouse) Invited
17:10-18:00	Lab. Tour
18:00-19:30	Mixer (IMR Lounge)

#### "SMS2019 & GIMRT User Meeting Program 2019" Nov. 27-28, 2019 Venue: Auditorium, IMR, Tohoku Univ.

## Workshops

#### "SMS2019 & GIMRT User Meeting Program 2019" Nov. 27-28, 2019 Venue: Auditorium, IMR, Tohoku Univ.

Nov. 28 (Th	u.) : Day 2
	Scientific Session III : Structural Mateials Chair: G. Miyamoto
09:00-09:30	"New Era of Metallurgy through High Entropy Alloys" H. S. Kim (Pohang Univ. of Science and Technology) Keynote
09:30-10:00	"Unique Mechanical Properties by Nano–Macro Synergy Effects in Harmonic Structure Designed Metallic Materials" K. Ameyama (Ritsumeikan Univ.) Keynote
10:00.10:20	"The Effect of Crystalline Defects on Transformation Crystallography in Mg Alloys" X. Gu (Univ. of Science and Technology Beijing) Invited
$10:20 \cdot 10:50$	Coffee Break
	Scientific Session IV : Energy Materials and Crystal Growth Chair: T. Wada
10:50-11:20	"Dealloyed Porous Materials for Advanced Batteries" M. Chen (Johns Hopkins Univ.) Keynote
11:20-11:40	"Thermoelectric Performance and Defect Studies of Compositionally Homogeneous Si <sub>1'x</sub> Ge <sub>x</sub> " M. Arivanandhan (Anna Univ.) Invited
11:40.12:00	"Diffusionless Isothermal Omega Transformation in Titanium Alloys: Thermodynamics and Kinetics of Displacive Phase Transition Driven by Quenched–in Compositional Fluctuations" M. Tane (Osaka Univ.) Invited
12:00.13:30	Lunch
	Scientific Session V : Quantum Beam and High Field Chair: S. Kimura
13:30-14:00	"Competition and Collaboration Are Key to Understanding High-Temperature Superconductors" J. Tranquada (Brookhaven National Lab.) Keynote
14:00-14:30	"Studying Collective States in Materials with Soft X-rays at High Magnetic Fields at BESSY II" E. Weschke (Helmholtz-Zentrum Berlin) Keynote
$14:30 \cdot 14:50$	"Development of Iron-based Wires and Tapes for High Field Applications" Y. Ma (Inst. of Electrical Engineering, Chinese Academy of Sciences) Invited
14:50.15:10	"Magnetic Field Induced Transitions in Multiferroic BiFeO <sub>3</sub> " M. Matsuda (Oak Ridge National Lab.) Invited
15:10.15:30	Coffee Break
Scienti	fic Session VI : GIMRT Activities Report from Young Researchers Chair: K. Yubuta
15:30-15:50	"Single Crystal Growth and Physical Properties of Unconventional Superconductor UTe2" A. Nakamura (Tohoku Univ.) Invited
15:50-16:10	"Structural Investigations on the Rejuvenation Effect by Thermal Strain in Metallic Glasses" J. Stellhorn (Hiroshima Univ.) Invited
16:10-16:30	"Computation of Phonon Related Transport Properties in Semiconducting Materials" E. Minamitani (Inst. for Molecular Science) Invited
16:30-17:00	Closing K. Sugiyama

Keywords: SMS, GIMRT ICC-IMR, Tohoku University E-mail: icc-imr@imr.tohoku.ac.jp

# Activity Report

Young Researcher Fellowships



Young Res	search Fellowshi	sd				
Application No.	Title	Applicant	Affiliation	Host Professor	Proposed Research	Term
19FS01	Post Doctoral Fellow	Tao Yu	Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands	Prof. Bauer	Chiral Thermal Pumping of Magnons	2019.7.31-9.13
19FS02	PhD Student	Stanislav Olegovich Shirshikov	National University of Science and Technology "MISiS", Russia	Prof. Kato	Microstructural and Magnetic Properties Study of HPT-Compacted FeCo Powders	2019.9.28-12.3
19FS03	PhD Student, Junior Researcher	Daniel Maslennikov	Institute of Solid State Chemistry and Mechanochemistry SB RAS, Russia	Assoc. Prof. Belosludov	Investigation of the Effect of Green GDC (Gd-Doped Ceria) Powder Morphology on the Properties of the Ceramics Sintered Using Different Techniques.	2019.7.6-8.20
19FS04	PhD Student	Andoni Zabala Lekuona	University of the Basque Country, Spain	Prof. Nojiri	Magnetic Characterization of Zn(II)-Ln(III) based Single Molecule Magnets (SMMs)	2019.10.8-11.9
19FS05	PhD Student	Sanu Mishra	CNRS and University of Grenoble Alpes, France	Prof. Aoki	High Quality Single Crystals Fermi Surface Studies on Ce-based Heavy Fermion Compounds	2019.7.30-10.2
19FS06	Ph.D. Student	Warut Chewpraditkul	King Mongkuťs University of Technology Thonburi, Thailand	Prof. Yoshikawa	Growth and Characterization of (Lu,Y,Gd) <sub>3</sub> (AI,Ga) <sub>5</sub> O <sub>12</sub> :Ce,Mg Crystals for Timing Application	2019.7.31-10.29
19FS07	Ph.D. Student	Mariana Carla Mendes Rodrigues	The University of British Columbia, Canada	Prof. Furuhara	Multi-Scale 3D Characterization of Two Phase Microstructure in Ti Alloys	2019.11.16-12.15

# Young Researcher Fellowships

#### Non-Contact Spin Pumping by Microwave Evanescent Fields

The angular momentum of evanescent light fields has been studied in nano-optics and plasmonics, but not in the microwave regime. We predict non-contact pumping of electron spin currents in conductors by the evanescent stray fields of excited magnetic nanostructures. The coherent transfer of the photon to the electron spin is proportional to the g-factor, which is large in narrow-gap semiconductors and surface states of topological insulators.

Efficient transfer of spin information among different entities is a key objective in spintronics. The electromagnetic field at frequency  $\omega$  carries a spin angular momentum density [1]

$$\mathcal{D} = \frac{1}{4\omega} \operatorname{Im} \left( \varepsilon_0 \mathbf{E}^* \times \mathbf{E} + \mu_0 \mathbf{H}^* \times \mathbf{H} \right)$$
(1)

where  $\mu_0/\epsilon_0$ are the vacuum permeability/permittivity, and in the microwave regime the magnetic field component dominates. The evanescent fields at boundaries can have local angular momentum with locked linear and angular momentum. The chiral electrical near-field a rotating electrical dipole, of e.g., unidirectionally excites surface plasmon polaritons [2]. Metallic striplines or coplanar waveguides biased by currents in the GHz regime also emit chiral magnetic near-fields, which is of considerable interest for magnonics, since chiral excitation is a robust and switchable mechanism that pumps a DC unidirectional magnon current by an AC field [3].

Spin pumping by exchange interaction is established when the magnet and conductor form a good electric contact [4], which is difficult to achieve between metals and semiconductors including graphene because of Schottky barriers and electronic structure mismatch. Even when a good contact to a magnet can be established, results may be difficult to interpret due to proximity effects. Spin pumping at a distance by microwaves solves these issues since it does not require direct contact between the magnet and the system of interest.

Here we address the non-contact angular momentum transfer to an electric conductor by stray magnetic fields emitted by an excited magnet, thereby generalizing the concept of spin pumping by a contact exchange interaction. We are motivated by the significant near fields that couple magnetic nanowires and ultrathin magnetic insulating films, causing several chiral magnon transport phenomena. We find that a magnetodipolar field pumps electron spins into a conductor in a non-chiral fashion without the need of an electric contact [4]. We illustrate the physics for a simple yet realistic model system of a magnetic nanowire on top of a two-dimensional electron gas (2DEG) as illustrated in Fig. 1. The latter may be graphene, but the effect is strongly enhanced by spin-orbit interaction, such as a large g-factor in InAs or InSb quantum wells (QWs) or the surface states of 3D topological insulator. The singularity of the spin susceptibility in a one-dimensional situation such as a carbon nanotube and Luttinger liquid recovers the chirality of the spin injection.



Fig. 1: Snapshot of spin pumping by the microwave dipolar field of an excited magnetic nanowire on top of a 2DEG. A thin tunneling barrier suppresses any exchange coupling. Orange arrows indicate the direction of the stray field.

#### <u>References</u>

- [1] K. Y. Bliokh and F. Nori, Phys. Rep. 592, 1 (2015).
- [2] J. Petersen, J. Volz, and A. Rauschenbeutel, Science **346**, 67 (2014).
- [3] T. Yu, Y. M. Blanter, and G. E. W. Bauer, Phys. Rev. Lett. 123, 247202 (2019).
- [4] Y. Tserkovnyak, A. Brataas, and G. E. W. Bauer, Phys. Rev. Lett. 88, 117601 (2002).
- [5] T. Yu and G.E.W. Bauer, arXiv:2001.08513.

Keywords: spintronics, electronic structure, spin current

Dr. Tao Yu (Max Planck Institute for the Structure and Dynamics of Matter Hamburg, Germany), E-mail: tao.yu@mpsd.mpg.de

### Young Researcher Fellowships

# The behavior of secondary phase in FeCo-based alloys subjected to high-pressure torsion.

In this work we investigating the influence of high-pressure torsion (HPT) on phase transformations, microstructure, magnetic properties and ordering of the FeCo-Ni, FeCo-Mo, and FeCo-Nb ternary alloys. The behavior of the different secondary phase precipitates under the HPT is of particular interest.

Severe plastic deformation techniques such HPT cause different as can phase transformations. Recently we investigated the effect of HPT-induced γ-phase suppression in FeCo-V ternary alloys [1]. Generally speaking, HPT process caused martensitic transformation with of γ-phase along non-equilibrium supersaturation of a bcc-type solid solution (aphase) in the FeCo-V alloy. HPT-induced supersaturation of the a-phase in FeCo-based alloys can be used for tailoring functional properties, such as coercivity and microhardness.

The goal of this research is to study the influence of HPT on microstructure, phase composition, atomic ordering and functional properties of the equiatomic FeCo-based intermetallic alloys.

Three alloys were selected for this research:  $FeCo_{(1-x)}-Ni_{(x)}$ ,  $FeCo_{(1-x)}-Mo_{(x)}$ , and  $FeCo_{(1-x)}-Nb_{(x)}$ . The concentrations of the ternary elements are selected with regard to a ternary phase diagram (in case of Ni) and previous studies [2] on solubility of ternary elements in FeCo. The alloys in form of cylindrical bars with a diameter of 10 mm were prepared by arc melting and tilt casting in Kato lab, IMR. Two series of the samples were prepared. In the first series the content of the third element was within or close to the solvability limit, in the second series the content exceeded the solvability limit. The samples were homogenised at 1000 °C for 1 hour under an argon atmosphere, to obtain nearly equilibrium state. x-ray diffraction was used to identify the phase composition after annealing (Cu Kα radiation). High-temperature solid solution type gamma-phase is clearly seen on the diffraction pattern of the FeCo-Ni20 alloy (Fig. 1) Due to high background noise from Fe-rich samples, it is hard to see the second phase in other diffraction patterns. However, second phase can be seen with an optical microscope. Fig 2 shows microhardness values, averaged over 10 measurements of each sample. Microhardness of FeCo-20at%Ni is the lowest, owing to the substantional amount of  $\gamma$ -phase. Other samples have elevetated values of HV, due to solid-state hardening and precipitation



Fig. 1 X-ray diffraction pattern of FeCo-X alloys after annealing.





HPT experiments in the Bridgman chamber followed by TEM, magnetic hysteresis measurements will be conducted in I. P. Bardin Central Research Institute of Iron and Steel Industry (Russia) and in National University of Science and Technology MISiS (Russia) shortly. We also planning to measure an atomic order degree by means of neutron diffraction.

#### **References**

 A.M. Glezer, D.V. Louzguine-Luzgin, L.F. Muradimova,
 S.O. Shirshikov, M.A. Libman, I.V. Shchetinin, N.S. Perov,
 D.L. Dyakonov, R.V. Sundeev, Intermetallics **115**, 106615 (2019)

[2] T. Sourmail, Prog. Mater. Sci., 50, 816–880 (2005)

Keywords: deformation, magnetic properties, phase transformation Full Name Shirshikov Stanislav Olegovich (National University of Science and Technology "MISiS") E-mail: keller1250@gmail.com

# Effect of the synthesis conditions of Ce<sub>0.9</sub>Gd<sub>0.1</sub>O<sub>1.95</sub> (10GDC) powder on its morphology and properties of oxygen-conductive ceramics obtained by spark plasma sintering (SPS).

In this work, two 10GDC powders were obtained by thermal decomposition of the same plate-like oxalate precursor under different reaction conditions. The powders with different morphologies were sintered using SPS. Electron microscopy was applied to investigate the ceramic samples obtained; their ionic conductivities were measured and compared.

Nowadays, Gd-doped ceria (abbr. GDC) is a material widely used as a solid electrolyte in solid oxide fuel cells (SOFC). High oxygen conductivity of GDC at intermediate temperatures 500-700°C is favorable for using it in SOFC. However, ceria powders poor sinterability usually possess that sophisticates manufacturing the materials. To improve the sintering of the powder, one can change its morphology or/and use non-conventional methods for sintering, for example, spark plasma sintering (SPS). In this work, 10GDC powders were obtained by thermal decomposition of the plate-like oxalate precursor Ce1.8Gd0.2(C2O4)3·10H2O. The synthesis procedure was analogous to that for  $Ce_2(C_2O_4)_3 \cdot 10H_2O$ , described in [1] but with addition 10 mol. % Gd(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O at the initial stage. This work aimed to investigate the influence of the thermal decomposition conditions on the 10GDC morphology and the properties of the ceramics sintered by SPS. The main factor that influenced the morphology was shown to be water vapor pressure during the dehydration stage (at 120°C). When it was high enough (Quasi-Equilibrium conditions), the crystalline intermediate product formed, and fragmentation of the crystal occurred. Otherwise, the crystal retained its shape and sizes (**pseudo**morph), forming a poorly dehydrated crystalized product. After oxidation of the two dehydrated products in air at 300°C, the powders of 10GDC-pseudo and 10GDC-QE were obtained (Fig.1, left). Peaks' positions in the PXRD pattern of each sample correspond to the fluorite structure (Fm3m). Crystallite sizes calculated from the peaks broadening were about 5-6 nm in each case that correlated with TEM data. However, the sizes and shape of the nanoparticle agglomerates tailored at the dehydration stage were different.



Fig. 1 Morphology of initial 10GDC powders and ceramics obtained by SPS.

The powders of 10GDC were compacted

### Young Researcher Fellowships

and sintered using SPS under the same conditions. Then the samples were annealed in air at 1200°C to oxidize samples and to get rid of the rest of carbon. The obtained ceramics were investigated by FEG-SEM (Fig.1, right). Unlike the 10GDC-pseudo sample, the 10GDC-QE sample obtained from the precursor dehydrated under high vapor pressure had no visible fractures. This sample also possessed much better values of ionic conductivity (2.07 S/m at 700°C) and the smaller activation energy (66 kJ/mol) (Fig.2). Thus, dehydration conditions of the chosen precursor were found to be an essential factor controlling morphology of 10GDC powder. Changing the powder morphology was shown to lead to obtaining ceramics with varied characteristics.



Fig. 2 lonic conductivity measurements on the 10GDC ceramic samples obtained.

#### References

 D.V. Maslennikov, A.A. Matvienko, S.A. Chizhik, A.A. Sidelnikov, Synthesis and structural characterization of ceria nanoparticle agglomerates with shape inherited from an oxalate precursor, Ceramics International. 45 (2019) 4137–4141.

Keywords: sintering, oxide, solid electrolyte Daniel Maslennikov (Corresponding author, Group of reactivity of solids, Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia) E-mail: daniel@solid.nsc.ru

#### Magnetic characterization of Zn(II)-Ln(III) based Single Molecule Magnets (SMMs)

Introductory part, Abstract: In order to fully characterize the dynamic magnetic properties of a wide number of SMMs, magnetization curves in a full cycle pulsed magnetic field were studied. This technique allows us to observe open hysteresis loops that are often undetectable with conventional measuring methods.

The SMMs studied in this period at IMR were previously characterized by the common alterning current (ac) magnetic measurements. This technique allows us obtaining relaxation times ( $\tau$ ) at different temperatures and, subsequently effective energy barriers ( $U_{eff}$ ) and  $\tau_0$  values. However, in our case due to the limitations of our instrument, these  $\tau$  values were obtained for high temperature ranges, over 10.0 K, a fact that becomes a problem when willing to study the quantum tunnelling regime (QTM), around 2 K.

A possibility to overcome this situation is to measure conventional hysteresis loops at low temperatures. However, it is well known that for low symmetry systems, the QTM is usually so strong that open loops are barely observed.[1] Thus, magnetization curves in a full cycle pulsed magnetic field were studied. These pulses are so strong and fast that even SMMs with strong QTM display open hysteresis loops, which allows us to compare similar compounds' behaviour in the low temperature range.

For instance, Fig. 1 shows open loops for compounds **1-4**. These coordination compounds are  $Zn_2Dy_2$  based tetranuclear systems with very similar core structures. They all contain a flexible Mannich H<sub>4</sub>L ligand with coordinating phenoxo, methoxy and amine groups (inset of Fig. 1 displays the structure of **1**, the other compounds are derivatives of it).



Fig. 1 Pulsed-field magnetization curves at 0.4 K. Inset: Molecular structure of **1**.

The first coordination sphere has been subtly modified by replacing the chelating nitrate with other ligands with different electron donating capacity. As observed in the figure, the steps occurring close to zero field differ from one to another, which clearly indicates that the modifications introduced in the structure are notably affecting the tunnelling regime.

Additionally, another family consisting of nine Zn(II)Dy(III) based compounds varying the bridging dicarboxylate was studied by the same technique. Apart from obtaining interesting information regarding the low temperature QTM, some of the systems displayed two thermally activated relaxation mechanisms (identified by two sets of maxima in the ac measurements), which were then detected in the pulsed-field magnetization curves. As an example, Fig. 2 shows the presence of two peaks for compound 5 in the dM/dB vs B plots, in fair agreement with the behaviour observed in ac magnetic measurements (molecular structure of 5 is depicted in the inset of Fig. 2).



Fig. 2 Differential of magnetization for compound **5** measured at 0.4 K. Inset: Molecular structure of **5**.

It is noteworthy that apart from the mentioned systems many others have been studied during the stay at IMR. The data is currently being analysed and the results are expected to be published in the near future. This work was supervised by Prof. H. Nojiri and Dr. I. F. Díaz-Ortega.

#### **References**

[1] I. F. Díaz-Ortega, J. M. Herrera, T. Gupta, G. Rajaraman, H. Nojiri and E. Colacio, Inorg. Chem. 56, 5594 (2017).

Keywords: lanthanide, magnetic properties

Full Name (Division Name or Affiliation): Andoni Zabala Lekuona (University of the Basque Country, UPV/EHU)

E-mail: andoni.zabala@ehu.eus

https://www.ehu.eus/es/web/gqiqa/bekadunak

#### Growth of High Quality Single Crystals of Cerium-Based Heavy Fermions and Their Lanthanum Analogs

Abstract: During the course of this work at ICC-IMR, using self-flux method, high-quality single crystal samples of Cerium-based heavy fermions were grown along with their non-4f reference analogs based on Lanthanum. Characterization measurements like EDX to establish the elemental composition and XRD to determine crystallographic orientations were are performed.

Cerium-based heavy fermions (HF) offer an amazing platform to study emergent physical phenomena like unconventional superconductivity, non-Fermi liquid behavior, quantum criticality and so on. Therefore, high quality samples of HFs are an utmost necessity to explore such interesting physics.

During my stay at ICC-IMR Japan, I tried to grow several samples of the popular Ce-based HF family, Ce<sub>m</sub>MIn<sub>3m+2</sub> (M = Rh, Co, Ir, Pt, Pd etc). In particular, the samples grown are the antiferromagnetic Ce<sub>2</sub>RhIn<sub>8</sub> [1], superconducting (SC) Ce<sub>2</sub>CoIn<sub>8</sub>[2], Ce<sub>2</sub>IrIn<sub>8</sub> that shows field-induced non-Fermi liquid behavior [3] as well as corresponding Lanthanum analogs, as shown in Fig 1.



Fig. 1 Single crystals of Ce-based heavy fermions and La analogs grown at ICC-IMR.

Ce<sub>2</sub>Coln<sub>8</sub> grew in mixed phase along with CeColn<sub>5</sub> while Ce<sub>2</sub>Coln<sub>8</sub> grew along with Celn<sub>3</sub>. Ce<sub>2</sub>Rhln<sub>8</sub> grew in single phase. EDX and XRD methods were employed for elemental characterization of these samples. Transport and thermodynamic properties of Ce<sub>2</sub>Coln<sub>8</sub> were determined as shown in figure 2.



Ce<sub>2</sub>Coln<sub>8</sub> becomes SC at a critical temperature ( $T_c$ ) ~ 0.45 K. Also, an enhanced Sommerfield coefficient ~ 0.75 J/K<sup>2</sup>mol was observed indicating heavy-fermion behavior as expected. Furthermore, observation of quantum-oscillations confirms high-quality of Ce<sub>2</sub>Coln<sub>8</sub> crystals. To thoroughly determine the Fermi-surface of Ce<sub>2</sub>Coln<sub>8</sub>, a dHvA study in high fields is planned in future.

However, Ce<sub>2</sub>IrIn<sub>8</sub> and Ce<sub>2</sub>RhIn<sub>8</sub> do not show any quantum oscillations in the dHvA effect up to 18 T. These systems also needs to be tested in high fields for quantum oscillations.

In summary, during the course of this stay, high-quality single crystals of heavy fermion systems were successfully grown which are vital to understand emergent physical phenomena.

#### **References**

A. L. Cornelius et al, Phys. Rev. B, **64**,144411 (2001).
 G. Chen et.al., J. Phys. Soc. Jpn. 71, 2836 (2002).
 J. S. Kim et al, Phys. Rev. B, **69**, 024402 (2004).

Keywords: Heavy Fermions, single crystals, superconductivity Sanu Mishra (LNCMI-CNRS, UGA, Grenoble France) E-mail: <u>sanu.mishra@Incmi.cnrs.fr</u> http://Incmi.cnrs.fr

# Growth and characterization of Gd<sub>3</sub>(Sc,Al,Ga)<sub>5</sub>O<sub>12</sub>:Ce and Gd<sub>3</sub>Sc<sub>2</sub>(Al,Ga)<sub>3</sub>O<sub>12</sub>:Ce,Mg multicomponent garnet crystals

he luminescence and scintillation characteristics of  $Gd_3(AI,Sc,Ga)_5O_{12}$ :Ce and  $Gd_3Sc_2(AI,Ga)_3O_{12}$ :Ce,Mg multicomponent garnet crystals grown by  $\mu$ -PD method are presented.  $Gd_3Sc_2Al_2GaO_{12}$ :Ce shows high RL yield 340% of BGO, LY of 24,000 ph/MeV and energy resolution of 9.5% at 662 keV  $\gamma$  rays.  $Gd_3Sc_2AIGa_2O_{12}$ :Ce shows faster scintillation decay time of 12 ns (12%). The acceleration of decay time and simultaneous decrease of its LY value are obtained for the Mg<sup>2+</sup>-codoped Gd\_3Sc\_2(AI,Ga)\_3O\_{12}:Ce,Mg samples.

Gd<sub>3</sub>Al<sub>2</sub>Ga<sub>3</sub>O<sub>12</sub>:Ce (GAGG:Ce) single crystal, prepared by the µ-PD down method, was discovered in 2011 and the first Czochralski - grown GAGG:Ce single crystal was reported one year later with high light yield (LY) of 46,000 ph/MeV [1]. Recently, an extremely high LY with fast scintillation decay time of about 90 - 120 ns were obtained for advanced GAGG:Ce crystals this work, investigate [2]. In we luminescence and scintillation properties of Gd<sub>3</sub>(Al,Sc,Ga)<sub>5</sub>O<sub>12</sub>:Ce and Mg-codoped multicomponent Gd<sub>3</sub>Sc<sub>2</sub>(Al,Ga)<sub>3</sub>O<sub>12</sub>:Ce by the garnet crystals grown micro-pulling-down method.

An example of as-grown GSAGG:Ce crystal is shown in Fig.1. The starting materials used were an 4N(99.99%) purity powders. An Ir crucible was used in the atmosphere of Ar + 2%O2 to prevent evaporation of gallium oxide.



Fig. 1 As-grown GSAGG:Ce crystal

The RL spectra of GSAGG:Ce crystals at RT in comparison with a BGO crystal are presented in Figs. 2. The integral scintillation efficiencies for the studied samples relative to a BGO (100%) reference



Fig.2 RL spectra of GSAG:Ce crystal ref. with BGO.

The LY(ph/MeV) and energy resolution ( $\Delta$ E/E) are collected under excitation with a <sup>137</sup>Cs source by coupling the crystals to an R6231 PMT. Gd<sub>3</sub>Sc<sub>2</sub>Al<sub>2</sub>GaO<sub>12</sub>:Ce shows highest LY value of 23,970 ph/MeV, LY value gradually decreased with increasing Ga/Al ratio.

PL decay of GSAGG:Ce samples measured at RT under excitation in the  $4f \rightarrow 5d1$ absorption of Ce<sup>3+</sup>. The shortening of PL decay time with the increasing Ga/Al ratio in the same trend with the decrease of RL yield and LY value. This can be explained by a larger thermal ionization from the 5d1 excited states to the conduction band.

#### **References**

[1] K. Kamada, T. Yanagida, T. Endo, K. Tsutumi, Y. Usuki, M. Nikl. J. Cryst. Growth 352 (2012).

[2] K. Kamada, S. Kurosawa, P. Prusa, M. Nikl, V. V. Kochurikin, T. Endo, K. Tsutsumi, H. Sato, Y. Yokota, K. Sugiyama, A. Yoshikawa. Opt. Mater. 36 (2014).

Keywords: Crystal growth, Luminescence, Scintillation

Warut Chewpraditkul (Department of Physics, Faculty of Science, King Mongkut's University of Technology Thonburi)

E-mail: Warut.chew@mail.kmutt.ac.th

#### Multi-scale 3D characterization of two-phase microstructure in Ti-alloys

Three dimensional (3D) characterizations were conducted in dual-phase Ti-Mo model alloys in order to gain insight into the microstructural aspects on meso and nano scales. Here, focused ion beam scanning electron microscopy (FIB-SEM) was used to characterize solid state phase transformation products. In the atomic scale investigations, the role that Molybdenum plays at the  $\alpha/\beta$  phase boundaries was studied by using 3D atom probe tomography (3DAPT).

Most titanium alloys used in aerospace and industrial applications consist of two-phase mixtures of  $\alpha$  and  $\beta$  phases combined in different arrangements [1]. Their relative volume fractions, distribution, size and morphology play a significant role in controlling the mechanical properties, which in turn, determine the in-service performance of the alloy [2]. Thus, it is industrially important and of considerable scientific interest to gain improved understanding of the microstructure development through the  $\beta \rightarrow \alpha$  phase transformation. Conventional microstructural characterization usina two-dimensional analysis mav provide insufficient information. Therefore, three dimensional microstructural investigations are often desirable for a more accurate bulk analysis.

In this study, a FEI Helios Nanolab 600i, focused ion beam scanning electron microscope, was used to investigate solid state phase transformation products, formed durina continuous cooling at 0.1°C/s in binary Ti-alloys with 2 and 6wt.% Mo additions. The 3D of microstructures reconstructions exhibit allotriomorphic  $\alpha$  and colonies of plate-like  $\alpha$ precipitates, called Widmanstätten structures, diffusion-controlled resulting from phase transformations at high temperatures, as shown in Fig. 1 for Ti-6wt.%Mo.



Fig. 1: 3-dimensional microstructural reconstruction of the Ti-6 wt.% Mo alloy.

A preliminary qualitative analysis shows a higher number of  $\alpha$  variants for Ti-6wt.%Mo as compared to Ti-2wt.%Mo. In addition, a significant reduction of  $\alpha$  plate thickness was observed with increasing Mo content, which can be related to the rejection rates of Mo from the  $\alpha$  phase.

3D atom probe tomography (3DAPT) was used to elucidate in more detail the effect of Mo on the  $\beta \rightarrow \alpha$  phase transformation kinetics. Here, a Ti-6wt.%Mo sample,  $\beta$ -solutionized and isothermally held at 800°C for 15 min prior to quenching, was investigated. 3DAPT needles were prepared in a FEI Quanta 200 3D microscope from an  $\alpha/\beta$  interface with a non-Burgers orientation relationship. 3DAPT analysis was performed on a Cameca LEAP 4000 HR system operating at a base temperature of 80K.

The Mo composition profile across the  $\alpha/\beta$ interface reveals a Mo partitioning into the  $\beta$ phase with concentrations ranging from ~6 to 7 at.%, whereas the  $\alpha$  phase is Ti-rich and only contains ~2 at.% Mo. While other elements appear to distribute homogeneously within the  $\alpha$ and β phases, a significant pile-up of Mo at the interface is observed. Such a preferential pile-up ahead of a growing  $\alpha$  phase can substantially decrease its growth rate. Moreover, it can also affect the local misfit between the  $\alpha$  and  $\beta$ and consequently phases influence the morphology of the  $\alpha$  precipitates [3].

Further analyses are yet to be conducted for a more comprehensive quantification of the effect of Mo on the  $\alpha$  formation kinetics and morphology.

#### **References**

[1] G. Lutjering and J.C. Williams, Titanium, 2<sup>nd</sup> Edition, Engineering Materials and Processes, Springer, 2007.

[2] J.D. Cotton, R.D. Briggs, R.R. Boyer, S. Tamirisakandala,P. Russo, N. Shchetnikov and J.C. Fanning, JOM (2015) 1281-1303.

[3] S. Nag, R. Banerjee, J.Y. Hwang, M. Harper and H.L. Fraser, Philos. Mag. 89 (6) (2009) 535-552.

#### Keywords: alloy, microstructure, morphology

Full Name: Mariana C. M. Rodrigues (The University of British Columbia) E-mail: mariana.rodrigues@alumni.ubc.ca https://www.grad.ubc.ca/unit/department-materials-engineering

### ICC-IMR FY2019 Activity Report

Edited by ICC-IMR Office Published in August, 2020

Contact: International Collaboration Center, Institute for Materials Research (ICC-IMR), Tohoku University Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan TEL&FAX: 81-22-215-2019 E-mail: icc-imr@imr.tohoku.ac.jp

Printing: HOKUTO Corporation



