



International  
Collaboration  
Center

Institute for Materials Research  
Tohoku University

# ICC-IMR FY2012 Activity Report

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



---

ICC-IMR FY2012

# Activity Report

---

**International Collaboration Center**

Institute for Materials Research  
Tohoku University



# CONTENTS



Mission	02
Committee Members	03
Visiting Scholars	05
Integrated Projects	13
Workshops	21
<b>KINKEN WAKATE</b>	<b>31</b>
Short-term Visiting Researchers	35
Young Researcher Fellowships	45



# Mission

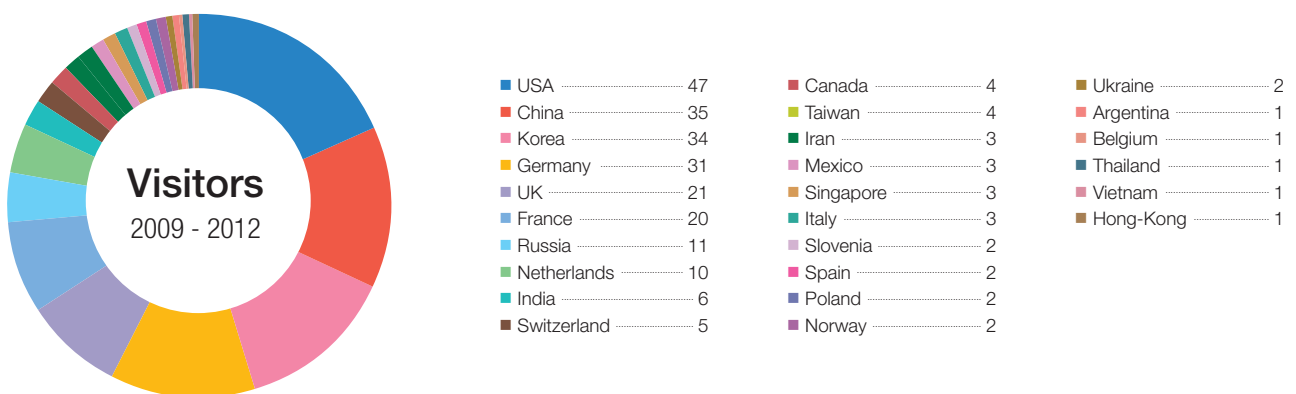
The ICC-IMR was founded in April 2008 as the center for international collaboration of the Institute for Materials Research (IMR) a center of excellence in material science, consisting of 27 research groups and five research centers. The ICC-IMR works as a gateway of diverse collaborations between overseas and IMR researchers. The ICC-IMR has invited 28 visiting professors and conducted 11 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 six different programs:

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

We welcome applicants from around the globe to submit proposals!

Visitors supported by ICC-Programs.



# ICC-IMR COMMITTEE MEMBERS

Director

Prof. Hiroyuki NOJIRI

Steering Committee

Prof. Takashi Goto

Prof. Koki Takanashi

Prof. Toyohiko Konno

Prof. Shin-ichi ORIMO

Prof. Eiji SAITOH

Prof. Gerrit E. W. BAUER





Activity Report

# Visiting Scholars



## FY 2012 Visiting Scholars

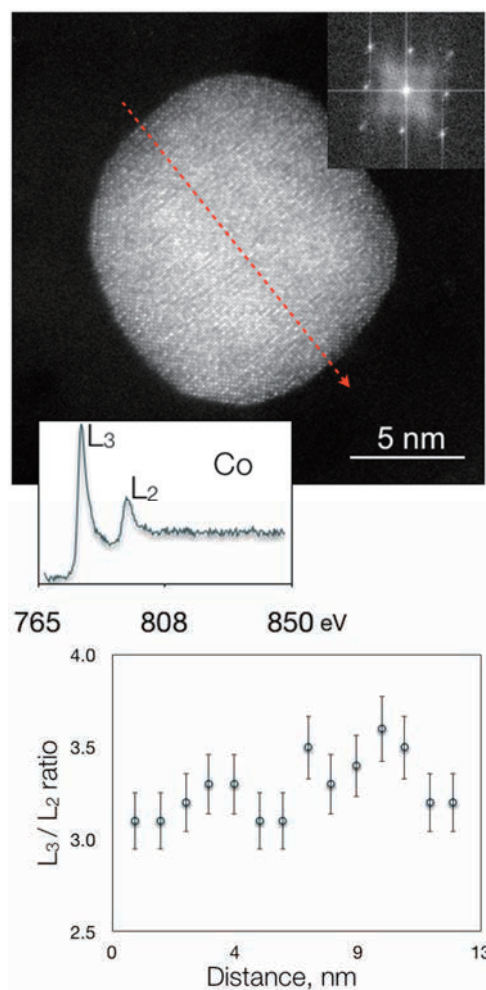
No.	Candidate	Host	Proposed Research	Title	Affiliation	Term
12G1	András Kovács	T. Konno	High-Resolution Chemical, Structural and Magnetic Study of Hard Magnetic Nanocrystals Using Advanced Electron Microscopy and Spectroscopy	Research Associate	Ernst Ruska Centre, Forschungszentrum Juelich, Germany	2012.11.22-2013.1.31
12G2	Donggyu Kim	T. Furuhashi	Hot Ductility Behavior of High Mn Steel with Various Deformation Conditions	Professor	Dong-A University, Korea	2012.6.1-7.31
12G3	Georges Boulon	A. Yoshikawa	Crystal Growth and Spectroscopic properties of Laser Single Crystals/ Ceramics	Emeritus Professor	CNRS and Institut Laue Langevin, France	2012.11.15-12.15

## High-resolution chemical, structural and magnetic study of hard magnetic nanocrystals using advanced transmission electron microscopy

*Understanding the magnetic properties of nanometer-sized  $L1_0$  crystals requires detailed structural, chemical and magnetic characterizations. In this work we studied soft and hard magnetic ( $L1_0$ ) alloys of Co-Pt nanocrystals [1] using high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) and electron energy-loss spectroscopy (EELS) techniques at the IMR.*

Magnetic nanocrystals have attracted much interest for future spintronics devices due to their unique magnetic and magnetotransport properties. Chemical properties such as alloy composition and chemical bonding as well as electron spin state can be elucidated using a combination of HAADF STEM and EELS methods. In this work we used energy-loss near-edge structure to determine the peak ratio of the L3 and L2 Co edges as a function of the nanocrystals size and chemical order. Aberration-corrected STEM was used in order to do the chemical characterization in high-spatial resolution. Co-Pt samples with different chemical composition and ordered states were studied. The Co-Pt nanocrystals were deposited using sequential electron beam deposition onto freshly cleaved NaCl substrates and covered by alumina in order to protect the surface from oxidation. The (S)TEM/EELS studies of as-deposited  $\text{Co}_{26}\text{Pt}_{74}$  nanocrystals showed an averaged L3/L2 Co peak ratio of 3.1 at the alloyed regions, however it revealed a thin CoO surface layer formation on the surface of Co that increased the peak ratio to 3.5. A homogenous chemical composition and a L3/L2 peak ratio of 3.3 were found in the annealed Co-Pt nanocrystals with the same composition. Co-Pt nanocrystals with  $L1_0$  structure showed an averaged L3/L2 peak ratio of 3.2. In order to validate the peak ratio determination of Co-Pt nanocrystals, we compared the results to pure Co and CoO that were used as references.

Future studies of the magnetic field distribution around the Co-Pt and Co-Fe-Pt nanocrystals using electron holography will be performed at the Forschungszentrum Jülich, Germany.



**Aberration-corrected HAADF STEM image of a  $\text{Co}_{26}\text{Pt}_{74}$  alloy nanocrystal. Inset is a fast Fourier transform pattern showing no structural ordering. Background subtracted Co L-edge is shown in the next image that was used to determine the L3/L2 peak ratio along the nanocrystal as marked by red arrow.**

### References

1. K. Sato, K. Yanajima and T.J. Konno, Philosophical Magazine Letters 92, (2012) 408

### Key words

Magnetic nanocrystals, transmission electron microscopy, electron energy-loss spectroscopy

### Contact to

András KOVÁCS (ER-C, PGI-5,  
Forschungszentrum Jülich, 52425 Germany)  
E-mail: [a.kovacs@fz-juelich.de](mailto:a.kovacs@fz-juelich.de)  
<http://www.er-c.org>

## Austenite Stabilization through Reverse Transformation and Intercritical Annealing in Medium Manganese Steel

Austenite stabilization through reverse transformation and intercritical annealing of 8 Mn steel was investigated. A minimum austenite grain size of 2  $\mu\text{m}$  was achieved with 5 cycle reverse transformation. Austenite stabilization was obtained in a short period of intercritical annealing of lean alloy of 8 Mn steel having small grain size, which is obtained by 5 cycles of reverse transformation.

Lean alloyed steel containing 5 to 8 wt. % manganese refers to as the third generation advanced high-strength steel (AHSS) comparing to the second generation AHSS which requires high manganese level for the stabilization of the fully austenitic structure. Third-generation AHSS developments are focusing on stabilizing retained austenite in an ultrafine ferritic matrix such as martensite or bainite. Although austenite stabilization is obtained through diffusion of interstitial carbon in most processing strategies, diffusion of substitutional elements such as manganese has also been shown to be effective. Significant austenite fractions resulting from prolonged holding (24hr, 1 week) at an intercritical temperature allowing for manganese partitioning from ferrite into austenite have been reported [1].

Austenite stability is increased not only with increasing austenite stabilization element such as Mn and C, but with reducing grain size and increasing dislocation density [2]. Repetition of austenite to martensite transformation through thermal cycling of rapid heating and quenching would results in fine grained structure [3]. The medium manganese content steel having fine prior austenite grain size which is obtained by reverse transformation, would results in stabilized austenite at room temperature in reduced time period when it experiences intercritical annealing, as the manganese atoms do not need to go far for achieving equilibrium concentration of austenite.

Fe-8Mn-0.2Mo-0.04C alloy was prepared by vacuum induction melting furnace. Cast slab was hot rolled to the thickness of 14mm(80% reduction) at 1200°C. Homogenization was carried out for 86.4ks at 1150°C in a vacuum furnace followed by water quenching. Solution treatment was performed for 1.8ks at 850°C followed by water quenching for obtaining initial microstructure having a lath martensite structure. For the reverse transformation cycle, the specimens were re-austenitized at 730°C for 60s and quenched. The reverse transformation cycle was repeated up to 5 times. Intercritical annealing was performed for 3.6ks at 600°C

followed by air cooling.

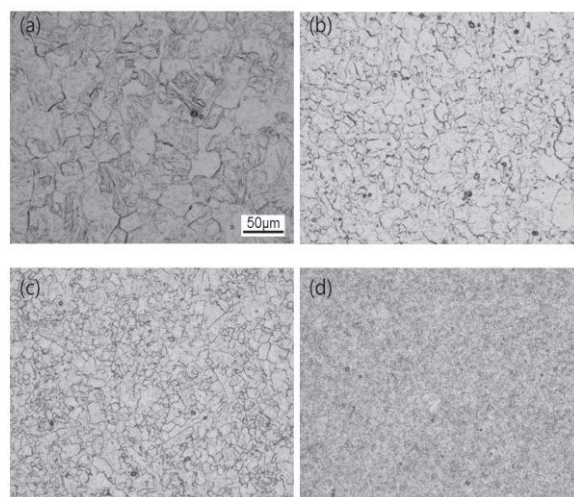


Fig. 1 Optical microstructures obtained by reverse transformation at 730°C. (a) 0 cycle; solution treated at 850°C for 1.8ks and followed by water quenching, (b) 1 cycle, (c) 2 cycle, (d) 5 cycle

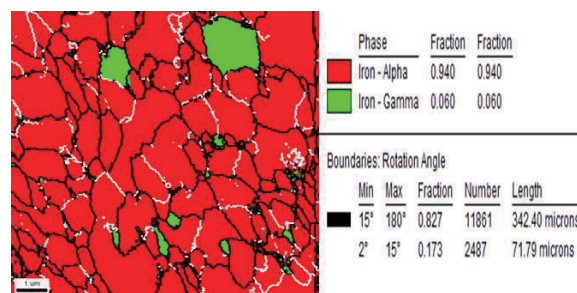


Fig. 2 EBSD phase map; 5 cycle reverse transformed at 730°C and followed by intercritical annealing at 600°C for 3.6ks.

Fig. 1 shows microstructures obtained by reverse transformation at 730°C. The initial austenite grain size is 26  $\mu\text{m}$ (Fig. 1(a)). Austenite grain size decreases with increasing thermal cycle. The austenite grain size decreases sharply after the first cycle, and finally prior austenite grain size 2  $\mu\text{m}$  was achieved with 5 cycles of reverse transformation.

Fig. 2 shows the EBSD phase map obtained from the intercritical annealing at 600°C for 3.6ks.

6 percent of the stabilized austenite was confirmed at room temperature with intercritical annealing of the specimen treated 5 cycle reverse transformation. The amount of stabilized austenite was reduced with decreasing reverse transformation cycle. It is thought to be due to the fact that the prior austenite grain size is decreased with reverse transformation cycle and resulting in the martensite structure having smaller packet and block sizes, thereby the distance need to move for achieving equilibrium concentration of austenite during intercritical annealing is reduced.

The results obtained in present work were summarized below.

A minimum austenite grain size of 2  $\mu\text{m}$  was achieved with 5 cycle reverse transformation. Austenite stabilization (6% austenite fraction) was obtained in a short period of intercritical annealing (600°C, 3.6ks) of lean alloy of 8 Mn steel having small grain size, which is obtained by 5 cycles of reverse transformation.

#### **References**

- [1] E. De Moor, D.K. Matlock, J.G. Speer and M. J. Merwin, Scripta Materialia, Vol. 64, 185 (2011)
- [2] S. Lee, S.J. Lee and B.C. De Cooman, Scripta Materialia, Vol. 65, 225 (2011)
- [3] T.Furuhara, K.Kikumoto, H.Saito, T.Sekine, T.Ogawa, S.Morito, T.Maki, ISIJ International, Vol. 48, 1038 (2008)

---

Keywords : Grain size, Phase Transformation, Steel  
Donggyu Kim (Dept. of Materials Science and Engineering, Dong-A University, Busan, Korea)  
E-mail: [dgkim@dau.ac.kr](mailto:dgkim@dau.ac.kr)  
<http://metal.donga.ac.kr>

## Title: Visiting Professor Research Subject. Crystal growth and spectroscopic properties of laser single crystals/ceramics

Abstract: I have continued fruitful cooperation with Pr.Yoshikawa and Pr;Goto Labs between November 13 and December 16, 2012, mainly on (Nd<sup>3+</sup>/Yb<sup>3+</sup>)-doped transparent sesquioxide and spinel ceramics or crystals for laser application. I also have been invited at the Material Science Week 2012, November 28 – 30, 2012.

This is a great privilege to cooperate with IMR Laboratories since a long time. I have proposed to apply our fruitful relationships between LPCML (nowadays ILM at the UCBLyon1) and IMR (Tohoku University) with the natural continuation of the laser materials research program on rare earth (Nd<sup>3+</sup>/Yb<sup>3+</sup>)-doped transparent sesquioxide and spinel ceramics/crystals as laser materials with high melting points. I want to express my acknowledgements to Prof. Niinomi, Head of IMR, Prof. Nojiri, Head of ICC-IMR, Prof. Konno, TEM Lab, Prof. Goto, SPS ceramics Lab and Prof. Yoshikawa, Advanced Crystal Engineering Lab.

The project ELYT lab : M12-LASMAT has started in march 2012, including Yoshikawa and Goto's teams. Lu<sub>2</sub>O<sub>3</sub> have been selected among sesquioxides for the following reasons: this is an un-active lattice in optics like Sc<sub>2</sub>O<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, the easy substitution of Lu<sup>3+</sup> by other rare earth cations as dopants, the highest thermal conductivity (12.5 W/m/K) and a lower phonon energy (391cm<sup>-1</sup>) comparing with YAG (700cm<sup>-1</sup>). We first focus our attention on Lu<sub>2</sub>O<sub>3</sub> ceramics, then we will study Lu<sub>2</sub>O<sub>3</sub> crystals grown by  $\mu$ -PD using a special crucible. Indeed, Lu<sub>2</sub>O<sub>3</sub> has high melting point up to 2490 °C, which makes it extremely difficult to be grown by conventional crystal growth methods. Such difficulties make people seek other ways to get Lu<sub>2</sub>O<sub>3</sub> as a ceramic laser material.

The research activity on advanced laser materials is

indeed increasing with the availability of transparent sintered polycrystalline ceramics which present some advantages compared to single crystals (sizes, mechanical strength, overall production cost, low cost) [1]. After the pioneer works of Dr. A. Ikesue [2] at the World Lab. Co.Ltd and Dr. H. Yagi at the Konoshima Company [3] on ceramics fabricated by conventional methods, an original and promising research is under progress, with the synthesis of Nd<sup>3+</sup>: Lu<sub>2</sub>O<sub>3</sub> ceramics by non-conventional Spark Plasma Sintering (SPS) technique by Prof.T. Goto's team [4]. The spectroscopic properties are analyzed at LPCML (UCBLyon1) and will be compared with the rare earth-doped crystals grown by Prof.A. Yoshilawa's team. Regarding the spatial distribution of rare earth dopants we have already published results with A. Yoshikawa's team on rare earth segregation phenomenon in YAG laser ceramics especially from TEM associated with EDX probe in cooperation with Dr. T. Epicier at INSA-Lyon lab [5-8]. We program the same evaluation with Lu<sub>2</sub>O<sub>3</sub> ceramic.

Another interest of Nd<sup>3+</sup>: Lu<sub>2</sub>O<sub>3</sub> single crystal is the recent report on laser output in 2011 [9] which points out a specific dual Nd<sup>3+</sup> wavelengths lasing at 1076.4 and 1080.5 nm (see Fig.1) very promising for applications in coherent terahertz (THz) generation by difference frequency and ultrahigh repetition rate pulse by optical beating.

Fabrication, thermal conductivity and structural

characterization by TEM will be done at IMR whereas spectroscopic and laser properties will be analyzed and optimized at ILM. Our first analysis of absorption spectra, emission spectra and life times of  $\text{Nd}^{3+} \ ^4\text{F}_{3/2}$  level under selective wavelengths made at LPCML(Lyon) have been submitted and discussed with the members of this cooperation.

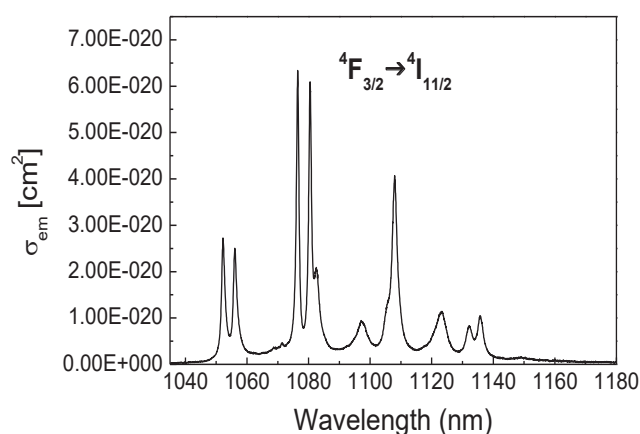


Fig.1 IR Emission spectra of 1%Nd-doped  $\text{Lu}_2\text{O}_3$  ceramic showing the two 1076.4 and 1080.5 nm laser lines of the main  $\text{C}_2$  crystallographic site.

It was also the opportunity to attend ICC-IMR- ELYT workshop on materials science on November 27 and to have been invited at the Material Science Week 2012 (MSW2012), Summit of Material Science, November 28– 30, 2012. The high interest of such Material Science Week is to have access to the large program of IMR on materials. My Invited talk was given for the Introduction session (I 2) and was related with "Laser materials: from single crystals to polycrystalline ceramics and distribution of rare earth dopants" which is directly

connected with my IMR cooperation [5-8]. The goal of this lecture was to present the evolution of laser materials from doped- single crystals to doped-ceramics. Another important cooperation between IMR (Prof. T Konno, Prof. K. Sato), INSA-Lyon (Dr. T. Epicier) and us in UCBLyon1 involves detection of Yb dopants at the atomic level in a YAG optical ceramic by STEM-HAADF, has been presented by T. Epicier (P 94).

## References

- [1] G. Boulon, *Optical Materials*, 34(3) (2012) 499-512
- [2] Ikesue, A.; Furusato, I.; Kamata, K. *J. Am. Ceram. Soc.* 78 (1995) 225–228.
- [3] J. Lu, M. Prabhu, J. Song, C. Li, J. Xu, K. Ueda, H. Yagi, T. Yanagitani, A. A. Kaminskii, *Jpn. J. Appl. Phys., Part 2* 40, L552 (2001)
- [4] L. An, A. Ito, T. Goto, *J. Amer. Ceramics Soc.* 94 (2011) 695-698 and 31(9) (2011) 1597-1602
- [5] W. Zhao, C. Mancini, D. Amans, G. Boulon, T. Epicier, Y. Min, H. Yagi, T. Yanagitani, T. Yanagida, A. Yoshikawa, *Jap. J. of App. Phys.* 49 (2010) 022602.
- [6] W. Zhao, S. Anghel, D. Amans, G. Boulon, T. Epicier, Y. Shi, X. Q. Feng, Y. B. Pan, V. Chani, A. Yoshikawa, *Optical Materials* 33 (2011) 684–687.
- [7] G. Boulon, T. Epicier, W. Zhao, V. I. Chani, T. Yanagida, A. Yoshikawa, *Jpn. J. Appl. Phys.*, 50, 9, Article ID: 090207, published on 2011/09/20 (online).
- [8] V. I. Chani, G. Boulon, W. Zhao, T. Yanagida, A. Yoshikawa, *Jpn. J. Appl. Phys.* 49 (2010) 075601
- [9] Liangzhen Hao and al. *Optics Express* 19, No. 18 (2011) 17774-17779

Keywords: Ceramic, laser, optical properties,  
 Full Name: Georges Boulon, Institute Light Matter (ILM), UCBLyon1-CNRS  
 E-mail: georges.boulon@univ-lyon1.fr  
<http://georges-boulon.univ-lyon1.fr>  
<http://ilm.univ-lyon1.fr>





Activity Report

# Integrated Projects



## FY2011-2012 Integrated Projects

No.	PI	Host	Proposed Research	Title	Affiliation	Term
11PJT1	Jürgen Schnack	H. Nojiri	Development of Functionalized Molecular-based Magnetic Materials	Professor	Bielefeld University, Germany	FY2011-2012
11PJT2	Yaroslav Tserkovnyak	G. Bauer	Theoretical Challenges in Spintronic Materials	Assoc. Professor	University of California, USA	FY2011-2012

## Development of functionalized molecule-based magnetic materials

**Abstract:** The main purpose of our integrated project was to explore new frontiers of molecular magnetism as well as to further improve our insight into molecule-based magnetic materials. We continued our synergetic strategy to combine the expertise brought into the group by scientists from three continents and a broad range of scientific fields as for example chemical synthesis, theoretical modeling and experimental investigation and manipulation.

**Magnetocalorics** aims at the development of new refrigerant materials based on magnetic molecules for sub-Kelvin refrigeration. In this very active field we could achieve a large number of impressive results. We obtained the largest magnetocaloric effect (MCE) reported so far for liquid-helium temperatures [A1] and designed one the very first examples of 3D molecule-based magnetic coolers containing Gd(III) [A2]. We investigated the role of the relative magnetic density in the MCE; this article was featured on the back cover of the Journal issue and selected as "VIP" paper [A3]. Other examples include lanthanide-free and cobalt-containing magnetic molecular refrigerants [A4-A13]. Extremely local coolers, i.e. cooling on the molecular level, could be designed by means of isolated molecules on surfaces [A14].

**Quantum computing** needs as an indispensable prerequisite long coherence times of the manipulated quantum states. Our investigations therefore focused on the synthesis and experimental investigation of promising new molecular magnetic qubits. By varying systematically each structural component of the molecular nanomagnet Cr<sub>7</sub>Ni, we identified and minimised the mechanisms of decoherence of the electron spin, thereby achieving a phase memory time exceeding 15 $\mu$ s at low temperatures [B1]. In order to couple several qubit-units chemical control of spin propagation between heterometallic rings was investigated [B2]. In a broader sense this addresses the issue of control of spin entanglement at the supramolecular level [B3-B5]. Phonons are one of the sources of decoherence; we investigated by means of NMR the decay of the time correlation function of molecular observables [B6]. From the theory point of view investigations of the time evolution are rather involved; some classical simulations are published in [B7].

**Single molecule magnets (SMM)** which

exhibit bistability and hysteretic behavior are candidates for next-generation storage devices. Within the project we follow routes of rational design of e.g. C<sub>3</sub>-symmetric molecular magnets in order to prevent losses through quantum tunneling and thus increase bistability [C1-C4].

**New magnetic molecules** have been synthesized, among them redox controlled magnetic {Mn<sub>13</sub>} Keggin systems (cover and "VIP") as well as a cyanide-bridged [CoFe] chain with three-way switching properties [D1-D17]. We could also demonstrate the first use of a flow system for the discovery of new cluster compounds and for the scale up of other cages previously only available in very small yields [D18]. Some of the large variety of theoretical modeling procedures are described in a chapter [D19] of a book on molecular magnetism which was edited by R.E.P. Winpenny.

**New experimental tools** such as four dimensional inelastic neutron scattering open new gateways to a better understanding of magnetic correlations [E1,E2]. Figure 1 shows the high intensity resolution that can be achieved in three dimensional Q-space[E1]. Together with modern EPR techniques [E3] such methods deliver a much more accurate picture of the internal magnetic structure than gross measurements such as magnetic susceptibility.

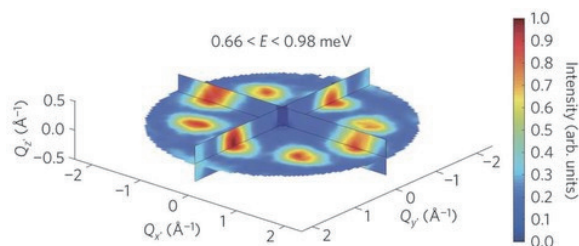


Fig. 1: Constant-energy plots of the neutron scattering intensity for a Cr<sub>8</sub> ring [E1].

**Deposition of magnetic molecules on surfaces** is a new scientific goal in order to be able to address single molecules by means of e.g. tunneling microscopy. Since many interesting molecules are fragile, and the details of the interactions with the surface are a priori unknown we first aimed at the control of self assembling of molecular rings on surfaces [F1-F4].

**Acknowledgment:** In the name of all participants of this integrated project I would like to thank IMR at Tohoku University for the generous support. Jürgen Schnack

## References

- [A1] G. Lorusso, J. W. Sharples, E. Palacios, O. Roubeau, E. K. Brechin, R. Sessoli, A. Rossin, F. Tuna, E. J. L. McInnes, D. Collison, and M. Evangelisti, *Adv. Mater.* (2013) - in press.
- [A2] G. Lorusso, M. A. Palacios, G. S. Nichol, E. K. Brechin, O. Roubeau, and M. Evangelisti, *Chem. Comm.* 48, 7592 (2012).
- [A3] M. Evangelisti, O. Roubeau, E. Palacios, A. Camón, T. N. Hooper, E. K. Brechin, and J. J. Alonso *Angewandte Chemie International-Edition* 50, 6606 (2011).
- [A4] E. Colacio, J. Ruiz, G. Lorusso, E. K. Brechin, and M. Evangelisti, *Chem. Comm.* 49, 3845 (2013).
- [A5] I. A. Gass, E. K. Brechin, and M. Evangelisti, *Polyhedron* 52, 1177 (2013).
- [A6] T. N. Hooper, J. Schnack, S. Piligkos, M. Evangelisti, and E. K. Brechin, *Angew. Chem. Int. Ed.* 51, 4633 (2012).
- [A7] F. Tuna, and R. E. P. Winpenny, *J. Amer. Chem. Soc.* 134, 1057 (2012).
- [A8] S. Sanz, R. D. McIntosh, C. M. Beavers, S. J. Teat, M. Evangelisti, E. K. Brechin, and S. J. Dalgarno, *Chem. Comm.* 48, 1449 (2012).
- [A9] S. K. Langley, N. F. Chilton, B. Moubaraki, T. Hooper, E. K. Brechin, M. Evangelisti, and K. S. Murray, *Chem. Sci.* 2, 1166 (2011).
- [A10] L. J. Batchelor, M. Sander, F. Tuna, M. Helliwel, F. Moro, J. van Slageren, E. Burzurí, O. Montero, M. Evangelisti, F. Luis, and E. J. L. McInnes, *Dalton Trans.* 40, 5278 (2011).
- [A11] G. Rigaux, R. Inglis, S. Morrison, A. Prescimone, C. Cadiou, M. Evangelisti, and E. K. Brechin, *Dalton Trans.* 40, 4797 (2011).
- [A12] Y.-Z. Zheng, M. Evangelisti and R. E. P. Winpenny, *Angew. Chem. Int. Ed.* 50, 3692 (2011).
- [A13] Y.-Z. Zheng, M. Evangelisti and R. E. P. Winpenny, *Chem. Sci.* 2, 99 (2011).
- [A14] V. Corradini, A. Ghirri, A. Candini, R. Biagi, U. del Pennino, G. Dotti, E. Otero, F. Choueikani, R.J. Blagg, E.J.L. McInnes and M. Affronte, *Adv. Mater.* 2013, 25, 2816-2820.
- [B1] C.J. Wedge, G.A. Timco, E.T. Spielberg, R.E. George, F. Tuna, S. Rigby, E.J.L. McInnes, R.E.P. Winpenny, S.J. Blundell and A. Ardavan, *Phys. Rev. Lett.* 2012, 108, 107204
- [B2] T.B. Faust, V. Bellini, A. Candini, S. Carretta, L. Carthy, D. Collison, R.J. Docherty, J. Kenyon, G. Lorusso, J. Machin, E.J.L. McInnes, C.A. Muryn, R. G. Pritchard, S.J. Teat, G.A. Timco, F. Tuna, G.F. Whitehead, W. Wernsdorfer, M. Affronte and R.E.P. Winpenny, *Chem. Eur. J.* 2011, 17, 14020-14030.
- [B3] G. Lorusso, F. Troiani, V. Bellini, A. Ghirri, A. Candini, S. Carretta, P. Santini, G. Amoretti, W. Wernsdorfer, G. Timco, R.E.P. Winpenny, M. Affronte, *J. Phys.: Conf. Ser.* 303 012033
- [B4] V. Bellini, G. Lorusso, A. Candini, T. B. Faust, G. A. Timco, W. Wernsdorfer, R. E. P. Winpenny, and M. Affronte, *Phys. Rev. Lett.* 106, 227205 (2011).
- [B5] T. B. Faust, F. Tuna, G. A. Timco, M. Affronte, V. Bellini, W. Wernsdorfer and R. E. P. Winpenny *Dalton Transactions Dalton Trans.*, 41, 13626-13631 (2012).
- [B6] E. Garlatti, S. Carretta, P. Santini, G. Amoretti, M. Mariani, A. Lascialfari, S. Sanna, K. Mason, J. Chang, P. Tasker, E. K. Brechin, *Phys. Rev. B*, 2013, 87, 054409.
- [B7] H.-J. Schmidt, C. Schröder, M. Luban, *J. Phys.: Condens. Matter* 23 (2011) 38600.
- [C1] V. Hoeke, E. Krickemeyer, M. Heidemeier, H. Theil, A. Stämmler, H. Bögge, T. Weyhermüller, J. Schnack, and T. Glaser, *Eur. J. Inorg. Chem.*, 2013.
- [C2] V. Hoeke, M. Heidemeier, E. Krickemeyer, A. Stämmler, H. Bögge, J. Schnack, A. Postnikov, and T. Glaser, *Inorg. Chem.*, 2012, 51, 10929-10954.
- [C3] V. Hoeke, M. Heidemeier, E. Krickemeyer, A. Stämmler, H. Bögge, J. Schnack, and T. Glaser, *Dalton Trans.*, 2012, 41, 12942-12959.
- [C4] V. Hoeke, K. Gieb, P. Müller, L. Ungur, L. F. Chibotaru, M. Heidemeier, E. Krickemeyer, A. Stämmler, H. Bögge, C. Schröder, J. Schnack, and T. Glaser, *Chem. Science*, 2012, 3, 2868-2882.
- [D1] N. Hoshino, F. Iijima, G. N. Newton, N. Yoshida, T. Shiga, H. Nojiri, A. Nakao, R. Kumai, Y. Murakami, H.

Oshio, *Nature Chem.* 2012, 4, 921-926.

[D2] G. N. Newton, S. Yamashita, K. Hasumi, J. Matsuno, N. Yoshida, M. Nihei, T. Shiga, M. Nakano, H. Nojiri, W. Wernsdorfer, H. Oshio, *Angew. Chem.* 2011, 50, 5716-5720.

[D3] M.L. Baker, G.A. Timco, S. Piligkos, J. S. Mathieson, H. Mutka, F. Tuna, P. Kozłowski, M. Antkowiak, T. Guidi, T. Gupta, H. Rath, R. J. Woolfson, G. Kamieniarz, R.G. Pritchard, H. Weihe, L. Cronin, G. Rajaraman, D. Collison, E.J.L. McInnes and R.E.P. Winpenny, *Proc. Nat. Acad. Sciences* 2012, 109, 19113-19118.

[D4] H.N. Miras, M. Sorus, J. Hawke, D.O. Sells, E.J.L. McInnes and L. Cronin, *J. Amer. Chem. Soc.* 2012, 134, 6980-6983.

[D5] F. Piga, F. Moro, I. Krivokapic, A.J. Blake, R. Edge, E.J.L. McInnes, F. Luis, M. Evangelisti, D.J. Evans, J. McMaster and J. van Slageren, *Chem. Commun.* 2012, 48, 2430-2432.

[D6] H.N. Miras, D. Stone, D.-L. Long, E.J.L. McInnes, P. Kögerler and L. Cronin, *Inorg. Chem.* 2011, 50, 8384-8391.

[D7] Lorusso, G. Corradini, V. Ghirri, A. Biagi, R. del Pennino, U. Troiani, F. Timco, G. Winpenny, R.E.P. Affronte, M., *Phys. Rev. B* 86, 184424 (2012).

[D8] R. Biswas, Y. Ida, M.L. Baker, S. Biswasa, P. Kara, H. Nojiri, T. Ishida and A. Ghosh, *Chem. Eur. J.*, 19, 3943-3953 (2013).

[D9] A. McRobbie, A.R. Sarwar, S. Yeninas, H. Nowell, M.L. Baker, D. Allan, M. Luban, C.A. Muryn, R.G. Pritchard, R. Prozorov, G.A. Timco, F. Tuna, G.F.S. Whitehead and R. E. P. Winpenny, *Chem. Commun.* 47, 6251 (2011).

[D10] M.L. Baker, S. Piligkos, A. Bianchi, S. Carretta, D. Collison, E. J. L. McInnes, H. Mutka, G. A. Timco, F. Tuna, H. Weihe, H. U. Güdel, and R. E. P. Winpenny, *Dalton Trans.* 40, 8533 (2011).

[D11] M.L. Baker, A. Bianchi, S. Carretta, D. Collison, R.J. Docherty, E.J.L. McInnes, A. McRobbie, C.A. Muryn, H. Mutka, S. Piligkos, M. Rancan, P. Santini, G.A. Timco, P.L.W. Tregenna-Piggott, F. Tuna, H.U. Güdel and R.E.P. Winpenny, *Dalton Trans.* 40, 2725 (2011).

[D12] Casson, C.A. Muryn, F. Tuna, J. Schnack, R. E.P. Winpenny, *Polyhedron* (2013) in print

[D13] K. Graham, F.J. Douglas, J.S. Mathieson, S.A. Moggach, J. Schnack, M. Murrie, *Dalton Trans.* 40 (2011) 12271-12276.

[D14] K. Mason, J. Chang, E. Garlatti, A. Prescimone, S. Yoshii, H. Nojiri, J. Schnack, P. A. Tasker, S. Carretta and E.

K. Brechin, *Chem. Commun.* 47 (2011) 6018-6020

[D15] R. S. Winter, J. Yan, C. Busche, J. S. Mathieson, A. Prescimone, E. K. Brechin, D.-L. Long, L. Cronin, *Chem. Eur. J.*, 2013, 19, 2976-2981.

[D16] K. Mason, J. Chang, A. Prescimone, E. Garlatti, S. Carretta, P. A. Tasker, E. K. Brechin, *Dalton Trans.*, 2012, 41, 8777-8785.

[D17] S. G. Mitchell, P. I. Molina, S. Khanra, H. N. Miras, A. Prescimone, G. J. T. Cooper, R. S. Winter, E. K. Brechin, D.-L. Long, R. J. Cogdell, L. Cronin, *Angew. Chem. Int. Ed.*, 2011, 50, 9154-9157.

[D18] C. J. Richmond, H. N. Miras, A. Ruiz de la Oliva, H. Zang, L. Paramonov, C. Makatsoris, R. Inglis, E. K. Brechin, D.-L. Long, L. Cronin, *Nature Chem.*, 2012, 4, 1307-1043.

[D19] L. Engelhardt, C. Schröder, "Simulating computationally complex magnetic molecules", in *Molecular Cluster Magnets* (Ed: R. E. P. Winpenny), World Scientific Publishers, Singapore, ISBN: 9-8143-2294-6 (2011); achievements: review of state-of-the-art simulational techniques for magnetic molecules research.

[E1] M.L. Baker, T. Guidi, S. Carretta, J. Ollivier, H. Mutka, H.U. Güdel, G.A. Timco, E.J.L. McInnes, G. Amoretti, R.E.P. Winpenny and P. Santini, *Nature Physics* 2012, 8, 906-911.

[E2] M.L. Baker, O. Waldmann, S. Piligkos, R. Bircher, O. Cador, S. Carretta, D. Collison, F. Fernandez-Alonso, Eric J. L. McInnes, Hannu Mutka, Andrew Podlesnyak, Floriana Tuna, Stefan Ochsenbein, Roberta Sessoli, Andreas Sieber, Grigore A. Timco, Hogni Weihe, Hans U. Güdel, and Richard E. P. Winpenny, *Phys. Rev. B.* 86, 064405 (2012).

[E3] Y. Oshima, H. Nojiri, J. Schnack, P. Kögerler, and M. Luban, *Phys. Rev. B*, 85, 024413 (2012).

[F1] Oxo-centered carboxylate-bridged trinuclear complexes deposited on Au(111) by a mass-selective electrospray. V. Corradini, C. Cervetti, A. Ghirri, R. Biagi, U. del Pennino, G. A. Timco, R. E. P. Winpenny and M. Affronte, *New Journal of Chemistry*. Volume: 35 Issue: 8 Pages: 1683-1689.

[F2] Self-assembled monolayer of Cr<sub>7</sub>Ni molecular nanomagnets by sublimation. A. Ghirri, V. Corradini, V. Bellini, C. A. Muryn, G.A. Timco, R.E.P. Winpenny and M. Affronte *ACS Nano.* 5 (9) 7090-7099 (2011).

[F3] V. Corradini, A. Ghirri, E. Garlatti, R. Biagi, V. De Renzi, U. del Pennino, V. Bellini, S. Carretta, P. Santini, G. Timco, R. E. P. Winpenny, and M. Affronte, *Adv. Func. Mat.* 22, 3706-3713 (2012).

[F4] H. Rath, G. A. Timco, V. Corradini, A. Ghirri, U. del Pennino, A. F. Lisardo, R. G. Pritchard, M. Affronte and R. E. P. Winpenny, *Chem. Commun.* 49, 3404 (2013).

---

Keywords: magnetism, magnetic properties, chemical synthesis, neutron scattering, molecular devices

Full Name: Prof. Dr. Jürgen Schnack, Bielefeld University, Germany  
E-mail: [jschnack@uni-bielefeld.de](mailto:jschnack@uni-bielefeld.de)  
<http://www.molmag.de>

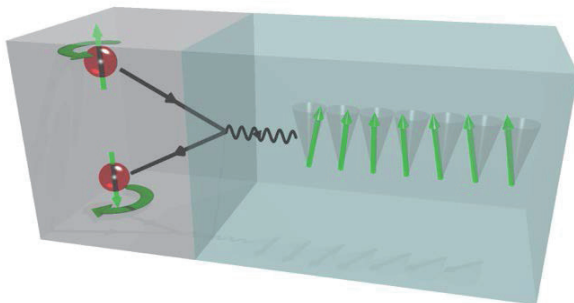
## Theoretical Challenges in Spintronic Materials

In the past two years we studied the theory of spintronics in the context of materials relevant for the experimental research at the IMR and elsewhere in the form of an ICC-IMR Integrated Project. The ICC-IMR helped to start up the new Theory of Condensed Matter Group to be integrated into the IMR environment and to enhance the international impact of IMR spintronics research.

In this project we addressed many issues of spintronics. For the present Activity Report we would like to present selected topics of our research into magnetic insulators, spin-pumping and spin Hall effects, as well as results obtained in the fields of spin caloritronics and spin optics.

### Magnetic insulators

The invention of thermal and electric actuation of the magnetic insulator Yttrium-Iron-Garnet by means of the direct and inverse spin Hall effect has attracted a lot of international attention. Fig. 1 is a sketch of the basic physical scattering process that couples the magnetization in insulators with metal electronics by spin momentum transfer that does not require charge transfer and is therefore operative as well for magnetic insulators.



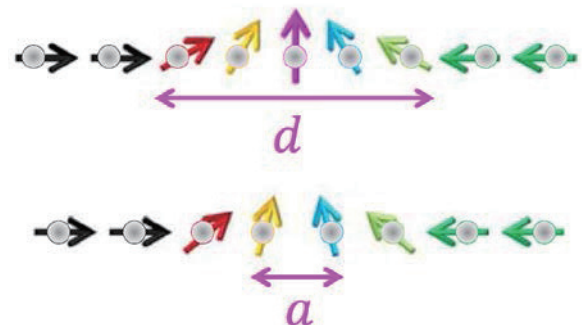
**Fig. 1:** The “bosonization of spintronics” rests on the magnon creation in magnetic insulators (right) by spin-polarized electron hole pairs or spinons (left).

In collaboration with the TU Delft and Fudan University with support by the ICC-IMR we studied various properties of YIG and its heterostructures. For example, we computed the critical currents for magnetic excitations (KINKEN Research Highlights 2012) and explained the recently discovered spin Hall magnetoresistance (SMR) that is described in the accompanying ICC-IMR research highlight.

### Spin caloritronics

Several recent experiments at the IMR and elsewhere discovered interesting spin effects in magnetic nanostructures, contributing to the field of spin caloritronics, the science and technology

of controlling charge, spin, and heat currents [1]. Theory has made progress by the qualitative elucidation of the basic mechanism of the spin Seebeck effect [1]. In the present project we continued to be active in this field, which led to results such as the domain wall heat conductance in magnetic insulators [2]. We found that the heat conductance is modulated by the magnetization texture when the domain wall width  $d$  becomes of the order of magnitude of the lattice constant  $a$  as illustrated in Fig. 2.



**Fig. 2:** Two head-to-head magnetic domain wall configurations with different energies illustrating the concept of atomic pinning for narrow domain walls when the domain wall width  $d$  becomes of the order of the lattice constant  $a$  [2]

### AC spin Hall effect

The spin current pumped by a precessing ferromagnet into an adjacent normal metal has a constant polarization component parallel to the precession axis and a rotating one normal to the magnetization. The former is now routinely detected as a DC voltage induced by the inverse spin Hall effect (ISHE).

In collaboration with the TU Delft we found AC ISHE voltages much larger than the DC signals for various material combinations and discuss optimal conditions to observe the effect [3]. The backflow of spin is shown to be essential to distill parameters from measured ISHE voltages for both DC and AC configurations. We believe that this backflow should have ramifications for other effect in ferromagnet-normal metal bilayers, such as the spin Seebeck effect.

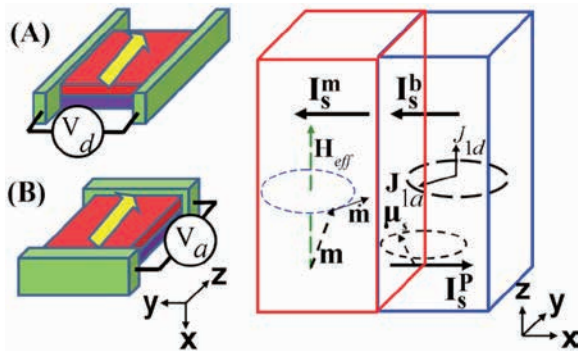


Fig. 3: Schematic spin battery operated by FMR for the measurement configurations (A) and (B). The AC(DC) voltage drops  $V_a$  ( $V_d$ ) along the  $z$ ( $y$ ) direction. In the right panel the magnetization  $\mathbf{m}$  (time derivative precesses around the effective field  $H_{eff}$  in the left layer, generating DC/ AC spin currents and a spin accumulation in the normal metal (right side) [3].

### Spin optics

Present magnetic storage technology is slow; switching of a bit takes of the order of a nanosecond, and switching by currents by use of the spin transfer torque does not appear to improve the switching speed much. A possible way out is the switching by light pulses, which can be very fast. Magnetization reversal by fs laser pulses has been demonstrated, but the basic physics has not yet been well understood. In collaboration with the NTNU Trondheim, Norway, we developed a theory for the light-induced magnetic fields in magnetic semiconductors [4], which are interpreted as a spin-dependent AC Stark effect. As result, we predict that at experimentally achievable light intensities effective magnetic fields of the order of 10's of tesla's can be realized.

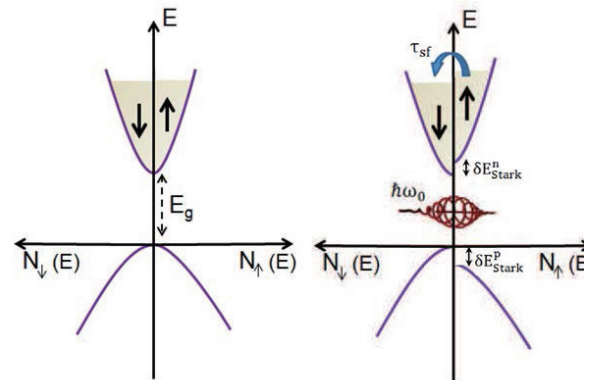


Fig. 4: Illustration of the changes in the majority and minority population due to the Stark shift in the presence of non-resonant and intense circularly polarized laser field that acts as an effective magnetic field to create a spin accumulation or exert torques on a magnetization [4].

### References

- [1] G.E.W. Bauer, E. Saitoh & B. J. van Wees, *Spin Caloritronics*, Nature Materials **11**, 391–399 (2012).
- [2] P. Yan and G. E. W. Bauer, *Magnonic Domain Wall Heat Conductance in Ferromagnetic Wires*, Phys. Rev. Lett. **109**, 087202 (2012).
- [3] H. Jiao and G.E.W. Bauer, *Spin backflow and AC Voltage Generation by Spin Pumping and Inverse Spin Hall Effect*, arXiv:1210.0724
- [4] A. Qaiumzadeh, G.E.W. Bauer, and A. Brataas, *Manipulation of Ferromagnets via the Spin-Selective Optical Stark Effect*, arXiv:1301.3481.

Keywords: magnetoresistance (transport), spin current, thermoelectricity  
 Gerrit E.W. Bauer (Theory of Solid State Physics, Institute for Materials Research, Tohoku University)  
 E-mail: . . . . g.e.w.bauer@imr.tohoku.ac.jp  
<http://www.imr.tohoku.ac.jp/en/org/research/01.html>



Activity Report

Workshops



## FY 2012 Workshops

No.	Chairperson	Title of Workshop	Place	Date
12WS1	E. Saitoh	Spin Caloritronics IV	Sendai	2012.6.2-6.5
12WS2	T. Goto	International Workshop on Biomaterials in Biosis-Abiosis Intelligent Interface Science	Zao, Miyagi	2012.8.2-8.3
12WS3	T. Matsuoka	Workshop on Nitride Semiconductors "Current Status and Future Prospects based on Intimate Discussion"	Sakura Hall, Tohoku University	2012.10.22-10.23
12WS4	H. Mizuseki	The 7th General Meeting of ACCMS-VO	IMR Lecture Hall	2012.11.23-11.25
12WS5	T. Konno	Advanced 0-D to 3-D Electron Microscopy: from the Detection of Single Atoms in Doped YAG to 3D Information on Functional Nanomaterials	TRUST CITY Conference, Sendai	2012.11.27
12WS6	K. Wagatsuma	Recent Advance in Analytical Techniques for Steelmaking Industry(RATEC2012)	Tokyo	2012.12.1
12WS7	H. Nojiri	International Workshop on Trends on Molecular Based Magnetic Compounds	IMR Lecture Hall	2013.2.18-2.21
12WS8	T. Goto	Japan-Russia Workshop on Advanced Materials Synthesis Process and Nanostructure	Zao, Miyagi	2013.3.7-3.8

## ICC-IMR International Workshop “Spin Caloritronics 4”

In the period of 2-5 June 2012 we organized an International Workshop on Spin Caloritronics, the 4<sup>th</sup> one in series held in Sendai and the Lorentz Institute of Leiden, see also <http://www-lab.imr.tohoku.ac.jp/~spincaloritronics4/>.

Spin caloritronics is the science and technology of the physical phenomena (and their control) associated with the coupling of charge, spin, and heat currents in nanoscale structures and devices [1]. This meeting was dedicated to reporting new results and general exchange of thoughts concerning the role of the electron's spin in the flow, control, and transformation of heat currents in (mainly) magnetic materials in order to add new functionalities and increase the efficiency of existing thermoelectric technology.

The Organizing Committee consisted of Stéphane Mangin (Nancy), Burkard Hillebrands (Kaiserslautern), Hideo Ohno (RIEC), Eiji Saitoh (IMR), Koki Takanashi (IMR), Kentaro Nomura (IMR), Saburo Takahashi (IMR), Gerrit Bauer (IMR) and Mika Terada (IMR secretary).

The Workshop gave an overview of spin caloritronics and our present understanding of the underlying physics. It covered all aspects of spin caloritronics, such as thermal spin injection, the spin-dependent Seebeck and Peltier effects in metallic nanostructures and tunnel junctions, the spin-Seebeck and spin-Peltier effects, thermal magnetization torques, thermal anomalous and spin Hall effects etc.. Theory, computations, and experiments were represented.

This was the 4<sup>th</sup> of a sequence of conferences that started in 2009 at the Lorentz Institute in Leiden, The Netherlands, followed by an ICC-IMR Workshop in 2010, and another one at the Lorentz Institute in 2011.

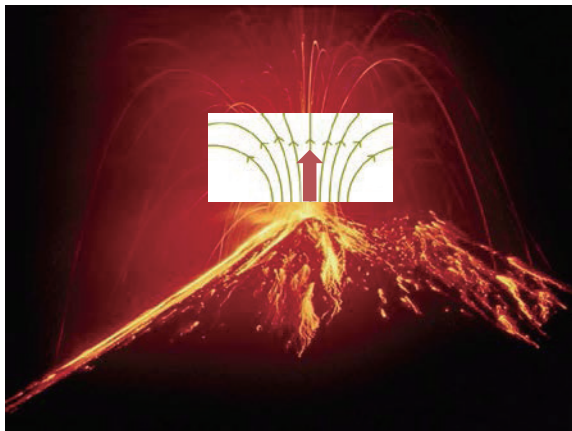


Fig. 1: Logo of Spin Caloritronics 4.

The large number (110) of participants from many different nations (see table) indicated the still growing interest in the topic. Several new and unpublished results were presented at the

workshop, such as the heat-current induced domain wall motion (Parkin) and the reduced damping in the free layer of a magnetic tunnel junction under a temperature difference (Schumacher).

The post session were integrated with the coffee breaks, which led to animated discussions of the posters during the whole workshop.

A 5<sup>th</sup> Workshop on Spin Caloritronics is planned to be held by Ohio State University in May 2013, while the 6<sup>th</sup> one will be organized by the DFG Priority Program in Kloster Irsee (Bavaria) in July 2014.



Fig. 2: Conference dinner with view on Matsushima Bay.

Country	# participants
Canada	2
China	1
France	2
Germany	16
Hong Kong	1
Japan	66
Korea	3
Netherlands	10
Saudi Arabia	1
Spain	1
Taiwan	1
United States	6

### References

[1] G.E.W. Bauer, E. Saitoh & B. J. van Wees, Nature Materials 11, 391–399 (2012)

Keywords: spintronics, thermoelectrics, spin current

Eiji Saitoh (Surface and Interface Research, IMR, Tohoku University)

E-mail: [eizi@imr.tohoku.ac.jp](mailto:eizi@imr.tohoku.ac.jp)

<http://www.imr.tohoku.ac.jp/>

## International Workshop on Biomaterials in Biosis-Abiosis Intelligent Interface Science

### -Innovative Research for Biosis-Abiosis Intelligent Interface Summer Seminar 2012-

Research on biomaterials has recently become crucial due to strong demands in developing materials for replacing human-body parts. The International Workshop on Biomaterials in Biosis-Abiosis Intelligent Interface Science (Innovative Research for Biosis-Abiosis Intelligent Interface Summer Seminar 2012) has provided a valuable forum for presentation, discussion, idea sharing, collaboration as well as interdisciplinary exchanges among the experts, researchers and students from different fields and expertise to meet and establish the intelligent interface science on biomaterials.

The Innovative Research for Biosis-Abiosis Intelligent Interface Summer Seminar 2012 was held on August 2 - 3, 2012 in Miyagi-Zao Royal Hotel, Miyagi, Japan as the first series of international forums in the frame of a 5-year research and collaboration project on Biomaterials in Biosis-Abiosis Intelligent Interface Science. The project involves 3 institutions, namely Institute for Materials Research, Graduate School of Dentistry, and Graduate School of Biomedical Engineering, Tohoku University. The financial support for the Summer Seminar was partly provided by International Collaboration Center-Institute for Materials Research (ICC-IMR), Tohoku University.

The Summer Seminar was held in a two-day technical program in which 24 papers were presented including 4 invited lectures by researchers of bio-/medical materials from Korea and the People Republic of China. About 48 participants consisting of experts, researchers and students attended the Summer Seminar. The invited speakers in this workshop were Prof. Zhixia Li (Dept of Chemical Eng., Guangxi University, China), Prof. Seog-Young YOON (School of Materials Science & Eng., Pusan National University, Korea), Prof. Jung-Suk HAN (School of Dentistry, Seoul National University, Korea) and Prof. Seong-Kyun KIM (School of Dentistry, Seoul National University, Korea).

The lecture by Prof. Z. Li was on the research on sol-gel derived magnetic microspheres for hyperthermia of cancer. Prof. S. Y. Yoon presented the study on in situ formation of biphasic calcium phosphates and their biological performance.

Meanwhile, Prof. J. S. Han's lecture was on the clinical use of alumina-toughened zirconia abutments for implant-supported restoration. Prof. S. K. Kim's presentation was on characterization of low-adherent bone marrow mesenchymal stem cells. Besides the invited lectures, numbers of papers on bio, dental and skeletal materials were presented by researchers and students.

The different academic backgrounds among the participants has provided the interdisciplinary exchange and enriched the viewpoints during the discussion of a specific topic. In addition, this workshop also accommodated researchers to have a good opportunity and forum to present their research in English as well as to touch the cutting edges of the development on biomaterials and innovative research for biosis-abiosis interface.



Fig.1. Participants of the International Workshop on Biomaterials in Biosis-Abiosis Intelligent Interface Science (Innovative Research for Biosis-Abiosis Intelligent Interface Summer Seminar 2012) in a photo session.

Keywords: biomaterials, biomedical, interdisciplinary collaboration

Contact to

Prof. Takashi GOTO

(Prof., Lab. of Multi-Functional Materials Science, Materials Processing and Characterization Division)

E-mail: goto@imr.tohoku.ac.jp

<http://www.goto.imr.tohoku.ac.jp/index.php>

## Find the way to go beyond the simple blue-light-emitting materials

The current status and difficulties which hinder the realization of high-crystal-quality group-III nitride alloy thin films and bulk crystals were assessed, and the way to solve these problems to open up novel device applications were intensively discussed. The critical importance of the strict trials on the crystal growth scheme was addressed, such as utilization of high-pressure, highly-nonequilibrium condition and exotic templates.

The international workshop "Intensive discussion on growth of nitride semiconductors" was held on October 22<sup>nd</sup>-23<sup>rd</sup>, 2012 in the Katahira Sakura Hall, Tohoku University. This workshop aimed to analyze the status quo, and to find the direction to take in the future and the problems that need to be solved in the field of nitride semiconductors.

Starting from the vapor-phase synthesis of GaN in 1969, the research on nitride semiconductors has progressed so that InGaN-based light emitting diodes and laser diodes in the visible wavelength regime are commercially available. In spite of these fruitions, however, the crystal qualities of these materials were still poor and have difficulties in the extension of the operating wavelength toward deep-UV and/or IR regimes with increasing the AlN and/or InN mole fractions, respectively. In particular the application of the semiconducting materials to novel devices operating at these extremely short and longer wavelengths were encouraged, in order to replace mercury gas tubes as well as conventional lasers by highly-luminescent emitters to meet the energy-saving policies of current world societies.

Based on the above targets, spirited 47 researchers from nine countries, most of them are crystal growers, gathered to share the problems such as immiscibility and lattice mismatch of nitride semiconductor thin films and bulk crystals. Numbers of novel techniques to improve the crystal quality have been spread out. Among all, in case of growth of alloy films with immiscible compositions, the precise control of in-plane stress by the adoption of pseudomorphic growth throughout the heteroepitaxial systems is expected to be useful to diminish the miscibility gap. This idea of intentional strain application has also been expanded to the unique idea, modulation of the electronic band profiles without impurity doping via piezoelectric effect, *i.e.* polarization doping, characteristic of the wurtzite crystals.

As for the trials on the alloy composition never achieved under thermodynamical equilibrium conditions with relevant growth apparatuses, the successful deposition of the volatile high-indium-content InGaN and InN films were reported by different groups: MOVPE growth under raised-pressure ambient up to 8 atm, droplet induced liquid-solid growth based on MBE as well as ultra-low-temperature pulsed sputtering deposition. As for the high aluminum content AlGaN, free standing AlN substrates grown by hydride vapor phase epitaxy and solid-source solution techniques are presented since the importance of the lattice-matched substrates has been stressed. Also the reduction of the threading dislocation density by selective area growth and use of the patterned substrates founds to be still applicable to the improve the performances of InGaN based devices, clearly shown by the successful realization quasi-step-free growth surface which is beneficial for obtaining high-quality quantum well structures.

The workshop chairs found a great deal of satisfaction in all the topics, and would like to say thank to all the panelists and participants who boosted the fruitful discussions.



Fig. 1 Taking a short break preventing the device failure due to the heating up.

Keywords: nitride, crystal growth, epitaxy  
Takashi Matsuoka (Physics of Electronic Material, IMR)  
E-mail: [matsuoka@imr.tohoku.ac.jp](mailto:matsuoka@imr.tohoku.ac.jp)  
<http://www.matsuoka-lab.imr.tohoku.ac.jp/>

## The 7<sup>th</sup> General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (ACCMS-V07) November 23–25, 2012, Chairperson H. Mizuseki (IMR)

The 7<sup>th</sup> annual meeting of “off the net” of the Virtual Organization (VO) for computational materials scientists mainly in the Asian region, who are working collaboratively daily via international computer network using our supercomputer at the Center for Computational Materials Science, Institute for Materials Research, Tohoku University (CCMS, IMR, TU) was held in IMR and Matsushima. This meeting focused on designing energy related materials and advanced methodologies in computational materials science, using the supercomputer at IMR and other member institutions aiming to use the Computer K in Kobe to perform ultra large scale simulation for new materials design. The details of the meeting and activities including photographs are open through our ACCMS webpage; please check <http://www-lab.imr.tohoku.ac.jp/~accmsvo/>.

Similar to the former 6 meetings, there were 21 invited, 26 oral, and 46 poster presentations, respectively with total 103 participants. The meeting is really international from 10 countries/regions. (This way of counting has been a tradition starting from the first meeting, suggested by the Chinese important members to solve complicated international relations.)

The meeting is not an international conference normally held by specific organization or on specific topic. This ACCMS-VO general meeting started based on the request by the members of the ACCMS to establish a Virtual Organization (VO, a terminology in computer science, which means a group of researchers whose official affiliations are different, but working daily using internet to communicate to achieve collaborative research.) We are very proud that the ACCMS-VO is a unique group started from IMR more than 10 years ago, which is composed of computational materials scientists in Asia, who are interested in international collaboration to encourage their research activity.

Therefore, the subjects are usually dispersed and mutual collaborations are dynamically arranged in the meeting time. However, this time, the 7<sup>th</sup> VO general meeting focused on energy related new materials, since this is one of the most urgent subjects in society, and many of the presentations were really related to this important topic and audience joined the discussion. As a tradition in all the meetings of ACCMS, 3 best posters are awarded to encourage young scientists for their future activity. This time, also 3 young researchers from Russia, Korea, and Japan were awarded the Kawazoe-Aida Prize.



Fig.1 One shot in a lecture, where attendants are freely discuss and communicate with the members in the ACCMS-VO to make future international collaborations.



Fig.2. Group photo of the attendants in the ACCMS-VO7 at the entrance of IMR.

Keywords: Computational Materials Science  
Hiroshi Mizuseki (IMR, Tohoku University)  
E-mail: [mizuseki@imr.edu](mailto:mizuseki@imr.edu)  
<http://www-lab.imr.edu/~accms/>

## Advanced 0-D to 3-D electron microscopy: from the detection of single atoms in doped YAG to 3D information on functional nanomaterials

Recent developments in transmission electron microscopy have proven to be one of the major thrusts in elucidating unsolved issues in materials science. This workshop hence served as an international platform for interactions among researchers in different disciplines, covering magnetic nanoparticles to optical ceramics, with common interests of making the best of modern microscopy techniques.

The main purpose of the workshop is twofold. First, we aim to elucidate the chemical and crystallographic structure of ceramic materials at the atomic level. Especially we have applied several characterization techniques, including Cs-corrected high-resolution TEM and atomic resolution STEM, in order to directly visualize the distribution of rare-earth dopant atoms in oxides for optical applications. Secondly, we intended to relate these structural characteristics of oxides to their physical properties, especially optical behaviors, such as absorption and fluorescence responses, and feedback them to the processing conditions,

Therefore, the participants and topics include Florent Tournus, INSA Lyon, France, ("Structure and magnetic properties of FeRh nanocrystals"), Martin Nikl, Institute of Physics, Czech Republic, ("Inorganic scintillation nanopowders and nanocomposites"), Christophe Dujardin, LPCML, Université Claude Bernard Lyon 1, France, ("Spatial distribution of luminescence in various systems), and Thierry Epicier, INSA Lyon, ("Atomic STEM studies by coupled HAADF

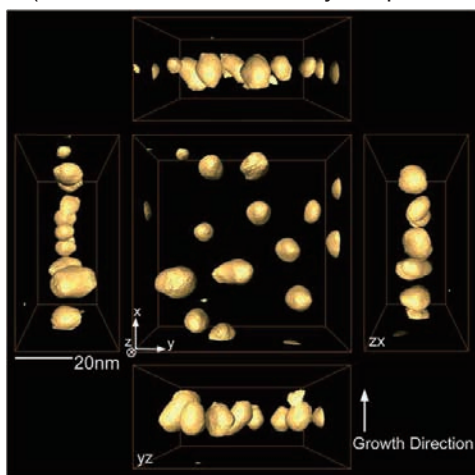


Fig. 1 3D tomographic images of magnetic nanoparticles

imaging and EELS chemical analysis"). Together with three presentations from IMR, from both processing and characterization points of views, discussions have been focused as to making the best usage of versatile but wide-ranging imaging and analytical techniques.

Figure 1 shows a distribution of FePd magnetic nanoparticles, reconstructed by SIRT method. As seen, three-dimensional feature is well visualized by using tomographic technique. However, a detailed analysis has disclosed non-negligible errors in the length estimation, especially in the z-direction.

Figure 2 shows STEM-HAADF image of a misfit

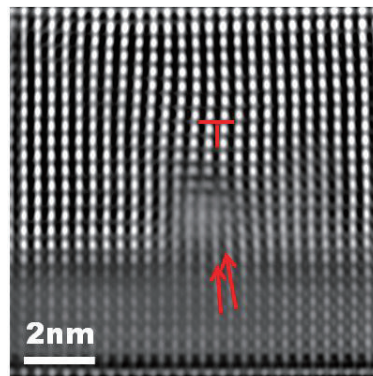


Fig. 2 STEM-HAADF image of SrTiO<sub>3</sub>-PbTiO<sub>3</sub> interface, showing a misfit dislocation.

dislocation at the bottom of a PbTiO<sub>3</sub> film deposited on a SrTiO<sub>3</sub> substrate. Distribution of strains within the film was quantitatively revealed by applying a strain analytical method, called geometrical phase analysis. This kind of defects acts as a source for 90° domain walls. [2]

### References

- [1] F. Tournus, K. Sato, T. Epicier, T.J. Konno, V. Dupuis, Phys. Rev. Lett. 110, 05501 (2013)
- [2] T. Kiguchi, K. Aoyagi, Y. Ehara, H. Funakubo, T. Yamada, N. Usami, T.J. Konno, Sci. Technol. Adv. Mater. 12, 034413 (2011)

## RATEC2012 -International Symposium on “Recent advance in analytical techniques for steelmaking industry

Ratec2012 was held in 2012. Nov. 28th-30th at National Museum of Emerging Science and Innovation (MIRAICAN), Koto-ku, Tokyo. There were 19 lectures, 19 poster presentations, and 56 participants. 10 foreign keynote speakers were invited from German, Belgium, Sweden, Australia, USA, China, and Korea.

The major objective of this conference is particularly that we can overview new trends of analytical techniques for process and quality controls in material industry, since they would contribute to the further development and production of new materials in various industry fields. Especially, the application of laser-induced breakdown spectroscopy (LIBS) for on-site/on-line elemental analysis was a remarkable topic, and we invite Dr. Prof. Reinhard Noll (Head of the Fraunhofer Institute for Laser Technology, Germany) and Dr. Victor Tusset (Head of the Advanced Techniques, Center for Research in Metallurgy, Belgium) to deliver a plenary talk about the recent advances of LIBS for quality control of steel products and for sorting of steel scraps according to their chemical compositions [1]. Other important topic of this conference is the microscopic observation techniques for the clarification of fine structure of materials. On this point, Dr. Andrey Karasev (KTH, Sweden) and other researchers made an excellent talk about the application of electrolytic extraction for investigation of inclusions and clusters in various steel grades and alloys on different stages of production [2]. The discussions with them were very heated, which resulted a foundation of connections each other.



Fig. 1 The plenary talk by Dr. ReinHard Noll, Head of the Fraunhofer Institute for Laser Technology, Germany

In this conference, we could show the presence of Japan's high research levels in the field of analytical science to especially the ICASI (International Committee of Analysis in Steel and Iron Industry) and CETAS (European Committee for the Study and Application of Analytical Work in the Steel Industry), and it is expected to hold such a kind of opportunity for ingathering of researchers to maintain and spread the presence. Finally, we truly acknowledge the financial support from International Corroboration Center, Institute for Materials Research (ICC-IMR).



Fig. 2 A scene during poster session.

### References

- [1] R. Noll, V. Strum, Ue. Aydin, D. Eliers, C. Gelhen, M. Hoehne, A. Lamott, A. Makowe, J. Vrenegor. *Spectochim. Acta. Part B: Atomic Spectroscopy*, 63, 10, 2008, pp.1159-1166.
- [2] S.Sato, Y. Arai, N. Yamashita, A. Kojyo, K. Komada, N. Ohtsu, Y. Okamoto, K. Wagatsuma. *Appl. Surh. Sci.*, 258, 2012, pp. 7574-7580.

Keywords: atomic emission spectroscopy, microstructure  
Full Name: Kazuaki Wagatsuma  
E-mail: [wagatsuma@imr.tohoku.ac.jp](mailto:wagatsuma@imr.tohoku.ac.jp)  
<http://wagatsuma.imr.tohoku.ac.jp/>



## Japan-Russia Workshop on Advanced Materials Synthesis Process and Nanostructure

Function and structure of materials strongly depend on their synthesis route. A new processing technique enables us to produce a novel material with a unique nanostructure. A precursor material also affects on the property and structure of products. This international workshop will focus on materials processing and precursor design for advanced materials synthesis.

Chemical vapor deposition (CVD) has been widely used for preparing films. CVD bulky plates, mainly non-oxides (nitrides and carbides) such as CVD-SiC wafer, have been prepared by CVD. Although oxides have useful applications for electronics, optics and protective coatings, CVD oxide thick films have hardly been obtained.

We have developed a new kind of laser CVD enabling high-speed and wide-area deposition by using high-power lasers [1]. The deposition rate of our laser CVD is several orders higher than those of conventional CVD. In addition, laser CVD films often had a unique nanostructure.

By using laser CVD, we have prepared various oxides and non-oxides films: thermal barrier coating of  $\text{Y}_2\text{O}_3\text{-ZrO}_2$  film with a feather-like structure containing a large amount of nano-sized pores which decreases the thermal conductivity [1], high-speed deposition of  $27500 \mu\text{m h}^{-1}$  for  $\text{SiO}_2$  coating [2], SiC-SiO<sub>2</sub> nanocomposite [3], highly c-axis oriented growth of  $\alpha\text{-Al}_2\text{O}_3$  film [4], a non-lead ferroelectric  $\text{BaTi}_2\text{O}_5$  film [5] and  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  superconducting film [6].

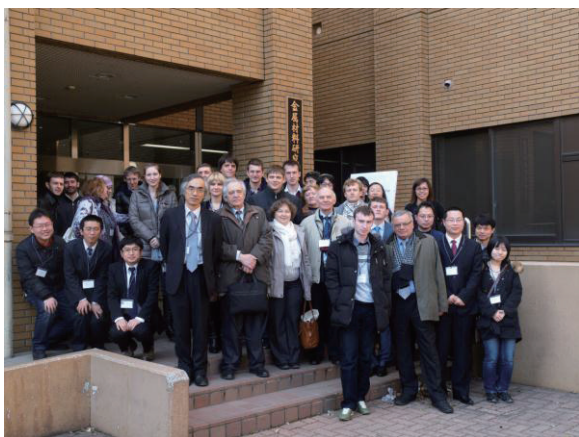


Fig. 1 A group photo at Japan-Russia CVD seminar held at IMR, Tohoku University.

Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences (NIIC SB RAS) has the advantages of producing novel and unique precursors for CVD process, such as for Si-N-C-N and B-C-N system. Methodology developed in NIIC SB RAS demonstrates preparations of CVD films for nanoscale electronic devices.

Tohoku University and SB RAS have a sufficient cooperative structure in many fields for a long time. Particularly, IMR and NIIC SB RAS both have strong potential in field of development of CVD processing. This collaboration will covers all steps of development of a novel CVD process: design and selection of new CVD precursor, establishment of their synthesis processes, thermodynamic modeling of CVD process, development of a new CVD utilizing auxiliary energy source, CVD coating at a wide range of conditions and characterization of processing-structure-properties relations.

Japan-Russia CVD seminar puts together researchers exchange ideas on cutting edge of CVD technology, and thus it is suitable for gain deep knowledge on advanced materials synthesis process. Joint workshop with excellent graduate schools in Tohoku University will encourage young researchers in Tohoku University, IMR and NIIC RAS through international interaction.

### References

- [1] T. Goto, Surf. Coat. Technol. 198, 367 (2005).
- [2] J. Endo, A. Ito, T. Kimura and T. Goto, Mater. Sci. Eng. B 166, 225 (2010).
- [3] S. Yu, R. Tu, A. Ito, T. Goto, Mater. Lett. 64, 2151 (2010).
- [4] Y. You, A. Ito, R. Tu and T. Goto, Appl. Surf. Sci. 256, 3906 (2010).
- [5] A. Ito, D.Y. Guo, R. Tu, T. Goto, J. Eur. Ceram. Soc. 32, 2459 (2010).
- [6] P. Zhao, A. Ito, T. Kato, D. Yokoe, T. Hirayama, T. Goto, Supercond. Sci. Technol. 26, 055020 (2012).

Keywords: nanostructure, alloy, thin film  
 Takashi Goto (Multi-Functional Materials Division)  
 E-mail: goto@imr.tohoku.ac.jp  
 http://http://www.excellent-materials.imr.tohoku.ac.jp/



Activity Report

KINKEN WAKATE



## FY 2012 KINKEN WAKATE

No.	Chairperson	Title of Workshop	Place	Date
12Wakate	K. Ohoyama	KINKEN WAKATE 2012 9th Materials Science School for Young Scientists and Students	IMR Seminar Room	2012.11.26

## KINKEN WAKATE 2012

### 9<sup>th</sup> Materials Science School for Young Scientists and Students

**K**INKEN WAKATE 2012, 9<sup>th</sup> Materials Science School for Young Scientists and Students, was held on 26<sup>th</sup>-November in 2012 in Institute for Materials Research. Four world's leading scientists were invited as lecturers, who gave excellent lectures about neutron and X ray scattering from basic introduction to some latest results.

KINKEN-WAKATE is an official annual event of Institute for Materials Research (IMR) since 2004. The attendees can learn advanced materials science and novel experimental techniques by experts' lectures. KINKEN WAKATE 2012 was held on 26<sup>th</sup>-November in 2012 in IMR, (Secretary: Dr. Ohoyama and Dr. Hayashi), organized by Center of Neutron Science for Advanced Materials Science, under full financial support of ICC-IMR. Four world's leading scientists were invited as lectures about introduction of neutron and X-ray scattering and its applications in novel materials science. Prof. Noda of Tohoku Univ. gave a excellent lecture about Introduction of Neutron and X ray scattering for material science. Prof. Jun'ichiro Mizuki, President of the Japanese Society for Synchrotron Radiation Research, gave a comprehensive lecture about material science in SPring-8, entitled "Introduction of Synchrotron Radiation X-ray Scattering - dynamics in materials and a proposal of marriage between X-rays and Neutrons- ". Dr. Seongsu Lee of Korea Atomic Energy Research Institute, Korea, gave a practical lecture about structural

investigations using neutron diffraction. Finally, Prof. Seunghun Lee of Univ. of Virginia, USA gave an impressive lecture about spin dynamics using neutron inelastic scattering.

19 young researchers attended, and enjoyed lectures and discussions in quantum beam science. In particular, in the night session, the attendants had beneficial opportunities to present their own investigations to the lecturers.



Fig.1 Discussion with Prof. Mizuki, President of the Japanese Society for Synchrotron Radiation Research



Fig.2 Lecture by Prof. Sunghun Lee (Univ. Virginia, USA) in his lecture about spin dynamics investigations by neutrons.

---

Keywords: Neutron Scattering, X-ray Scattering  
 Neutron Center of Advanced Materials Science  
 E-mail : imr\_neutron@imr.tohoku.ac.jp  
<http://neutron-center.imr.tohoku.ac.jp/index.html>



Activity Report

# Short-term Visiting Researchers



## FY 2012 Short-term Visiting Researchers

Application No.	Name	Host	Proposed Research	Title	Affiliation	Term
12SV1	Subhankar Bedanta	K. Takanashi	Magnetization Reversal Processes in Perpendicularly Magnetized FePt Dots	Assistant Professor	National Institute of Science Education and Research (NISER), India	2012.5.31-7.1
12SV2	Kwang-Yong Choi	H. Nojiri	Magnetization and ESR Investigation of the Decorated Shastry-Sutherland System $CdCu_2(BO_3)_2$	Associate Professor	Chung-Ang University, Korea	2012.6.20-6.28
12SV3	Hyung-Seop Shin	S. Awaji	Electro-Mechanical Property Evaluation in HTS CC Tapes Under Magnetic Field	Professor	Andong National University, Korea	2012.12.5-12.11
12SV4	Matej Pregelj	H. Nojiri	Antiferromagnetic Rsonance in Novel Frustrated Low Dimensional Magnetic Materials	Research Assistant	Jožef Stefan Institute, Slovenia	2013.1.13-1.23
12SV5	Georges Boulon	A. Yoshikawa	Development of Transparent Ceramics Superior to Single Crystal for High Power Laser Application	Emeritus Professor	Université Claude Bernard Lyon 1, France	2013. 2.12-3.3
12SV6	Takuya Yamamoto	K. Nagai	Embrittlement Trend Curve Prediction of Reactor Pressure Vessel Steels	Research Engineer	University of California Santa Barbara, USA	2013. 3.9-3.22
12SV7	Stefano Deledda	S. Orimo	Synthesis of Novel Complex Hydrides with Mixed Non-Metal-Based Complex Anions	Senior Scientist	Institute for Energy Technology (IFE), Norway	2013.3.1-9



## Magnetization reversal processes in perpendicularly magnetized FePt dots

We study the magnetization reversal processes in perpendicularly magnetized FePt continuous films and microfabricated dots. Understanding of different mechanism of magnetization reversal is very important for practical applications such as magnetic information storage or non-volatile magnetic random access memory (MRAM). We study the magnetization reversal process by magnetic force microscopy and Kerr microscopy.

$L1_0$ -ordered FePt ( $L1_0$ -FePt) is one of the promising hard magnetic materials to develop the ultrahigh density magnetic recording and large-scale integrated spintronic devices. In order to reveal the magnetization reversal mechanism of  $L1_0$ -FePt in a nanometer region, we investigate the magnetization reversal process in perpendicularly magnetized  $L1_0$ -FePt continuous films and microfabricated dots.

$L1_0$ -FePt thin films with different thicknesses were prepared by sputter-deposition. The Microfabrication of FePt nanodots was performed by e-beam lithography followed by ion beam milling. Nanodots of various diameters such as 500nm, 100nm, 30 nm with various center-to-center distances (pitch) were fabricated successfully. Triangular shaped dots of various lengths such as 100 nm and 30 nm were also fabricated. A few designs also have the honey comb structure. Scanning electron microscopy (SEM) was performed in order to measure the diameter or length of nanodots or nano-triangles. From the SEM images, it was confirmed that the dots were well separated and no surface to surface contact was observed ruling out the possibility of any direct exchange coupling between the FePt nanodots.

Magneto-optic Kerr effect (MOKE) magnetometry in the polar geometry was performed on all the FePt thin films as well as on the nanodot patterns. From the PMOKE loops we notice that the coercivity increases when the diameter of the dots are decreased. Also designs with the same diameter of dots but smaller pitch showed decrease in coercivity which indicates magnetostatic coupling mainly of dipolar nature between the dots. Dynamic MOKE hysteresis measurements where the sweep rate is varied have been performed on the FePt thin films as well as the nanodots. Figure 1 shows the dynamic magnetization hysteresis loops of a FePt thin film with the thickness of 5 nm. We have clearly observed that the coercivity increases as the frequency of measurement

increases, indicating the main contribution of domain wall motion as usually observed in ultrathin ferromagnetic thin films. Also magnetic force microscopy (MFM) has been carried out and the collective magnetization reversal processes in the ensembles of the FePt dots has been observed as a function of magnetic field, which is shown in Fig. 2. These results obtained from PMOKE and MFM will be compared with Kerr microscopy images, which is expected to find the existence of any domains consisting of a few FePt dots. [1]

### References

[1] S. Bedanta, T. Seki, T. Shima, and K. Takanashi (Unpublished).

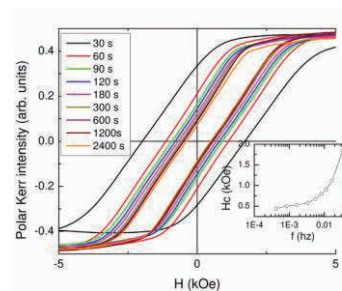


Fig. 1 Dynamic magnetization hysteresis loops of a FePt (5nm) thin film measured by PMOKE.

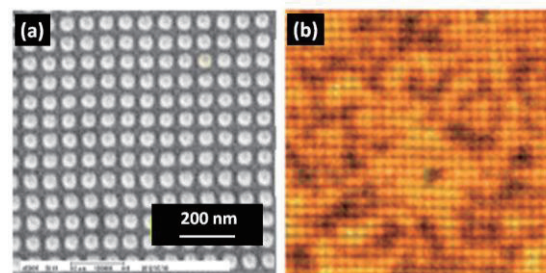


Fig. 2 (a) SEM and (b) MFM images of 25 nm FePt dots with the pitch of 75 nm. The MFM image was observed at  $H = -3$  kOe.

Keywords: magnetic nanostructure, magnetic properties  
 Dr. Subhankar Bedanta, Reader F, NISER, Bhubaneswar, India-751005  
 E-mail: sbedanta@niser.ac.in  
<http://www.niser.ac.in/~sbedanta/>

## Magnetization and ESR studies of $\text{Cd}(\text{Cu}_{1-x}\text{Zn}_x)_2(\text{BO}_3)_2$

We have investigated the magnetic properties of  $\text{Cd}(\text{Cu}_{1-x}\text{Zn}_x)_2(\text{BO}_3)_2$  ( $x=0, 0.1$  and  $0.2$ ) using high field magnetization and high frequency ESR in IMR. The Zn-substitution and field dependence of the magnetization and antiferromagnetic resonance modes suggest a competition between intradimer and inter-tetramer couplings.

$\text{CdCu}_2(\text{BO}_3)_2$  has attracted research interest as a counterpart of the well-investigated Shastry-Sutherland compound  $\text{SrCu}_2(\text{BO}_3)_2$  [1]. In contrast to  $\text{SrCu}_2(\text{BO}_3)_2$ ,  $\text{CdCu}_2(\text{BO}_3)_2$  has a long-range magnetic ordering at  $T_N=9.8$  K [2]. It is related to the fact that the substitution of  $\text{Sr}^{2+}$  by  $\text{Cd}^{2+}$  induces a structural transformation while changing a magnetic structure to a spin tetramer.  $\text{Cu}(1)\text{O}_4$  plaquettes form structural  $\text{Cu}(1)_2\text{O}_6$  dimers while tetrahedrally distorted  $\text{Cu}(2)\text{O}_4$  plaquettes share a common O atom with the dimers, forming a spin tetramer. The tetramer consists of strong intradimer coupling and weak intra- and inter-tetramer couplings. Thus, this compound offers a test bed to study a competition between a singlet state and a long-range ordered one in a single sample.

Fig.1 shows the high-field magnetization curve of  $\text{Cd}(\text{Cu}_{1-x}\text{Zn}_x)_2(\text{BO}_3)_2$  ( $x=0, 0.1$  and  $0.2$ ) measured at  $T=1.5$  K. The magnetization of  $x=0$  increases quasi-linearly with increasing field and exhibits a half-step magnetization plateau at  $H_{1/2}=22.4$  T and a spin-flop transition at  $H_{SF}=1.69$  T. In the 1/2-plateau phase, the spin dimer recovers a spin singlet state while other two tetramer spins are polarized parallel to the external field.

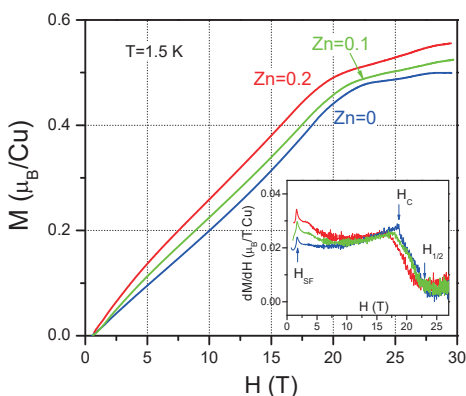


Fig. 1 Magnetization curve of  $\text{Cd}(\text{Cu}_{1-x}\text{Zn}_x)_2(\text{BO}_3)_2$ .

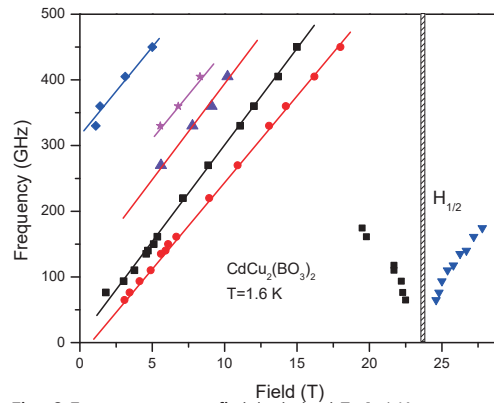


Fig. 2 Frequency vs. field plot at  $T=1.6$  K

With increasing Zn content to  $x=0.2$ , both  $H_{SF}$  and  $H_{1/2}$  are reduced by 15%, and the magnitude of the magnetization is systematically enhanced. This is due to a weakening of inter-tetramer coupling and a creation of free spins by dilution effects.

Fig. 2 shows the frequency-field plot at  $T=1.6$  K. We observe five modes which are assigned to the antiferromagnetic resonance modes pertaining to a four sublattice of the spin tetramer. In addition, one low-lying mode appears in the vicinity of the critical field  $H_{1/2}$ . This is ascribed to the magnetic field induced polarized phase.

In summary, the Zn-substitution and field dependence of magnetic behaviors rely on the peculiar spin arrangement comprising the strongly coupled  $\text{Cu}(1)$  dimer spins and the weakly coupled  $\text{Cu}(2)$  tetramer spins. The half-step magnetization and its Zn dependence is largely determined by the polarization and dilution effects of the  $\text{Cu}(2)$  spins, respectively.

### References

- [1] S. Miyahara and K. Ueda, J. Phys.: Condens. Matter 15, R327 (2003).
- [2] O. Janson et al., Phys. Rev. B. 85, 064404 (2012).

Keywords: High magnetic field, electron spin resonance, magnetic properties  
 Kwang-Yong Choi (Department of Physics, Chung-Ang University)  
 E-mail: kchoi@cau.ac.kr  
<http://www.quantummagnet.cau.ac.kr/>

## Electromechanical property evaluation in REC-DR GdBCO CC tapes under external magnetic field

Due to its promising potentials especially its low magnetic susceptibility, REBCO superconducting tapes attracts the attention of many potential applications such as power cables, motors and generators. In such applications, CC tapes were exposed to different stresses and strains from fabrication to operation. To achieve good designs of coils, the strain dependence of the critical current,  $I_c$  must be well understood. Therefore, electromechanical property evaluation of the CC tapes under magnetic field was conducted.

The design process of coils requires the understanding of the strain dependence of the critical current in the conductor and the ability to predict the strain state of the conductors in the coil. To ensure the performance of coated conductors in coil application, the evaluation of the electromechanical property under magnetic field is necessary and is one of the foremost things to do prior to device designing [1,2].

Coated conductor tapes sample fabricated using the reactive co-evaporation by deposition and reaction commonly known as RCE-DR were investigated in this study. The samples adopted the Hastelloy and stainless steel substrate, respectively. Moreover, they were brass laminated for further mechanical protection.

The samples were mounted on the Katagiri-type loading fixture for the evaluation of the electromechanical properties under different magnetic field intensities as shown in Fig. 1. In this manner, the magnetic field was applied in a perpendicular direction with respect to the CC tape's surface (B//c-axis). Magnetic field was produced by the 10 T cryo-cooled superconducting magnet at the HFLFM, IMR Tohoku University. The sample length, gauge

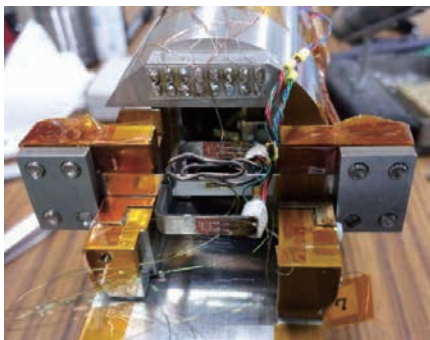


Fig. 1 CC tape sample mounted on the Katagiri-type tensile loading rig with double extensometer and strain gauges attached on the sample for sensing strain.

length and voltage tap separation used were 40, 20 and 10 mm, respectively. While critical current  $I_c$ , was measured using the four-probe method by 1  $\mu\text{V}/\text{cm}$  criterion.

The RCE-DR CC tapes with Hastelloy substrate was initially improved from 0 T up to 1 T which shows reduced strain sensitivity as shown by the representative curve of brass laminated CC tape in Fig. 2. However, increasing the magnetic field further to 3 T made the  $I_c$  behaved strain sensitive. Also, it was observed that a minimal  $I_c/I_{c0}$  peak strain existed at 1 Tesla. These behaviors of  $I_c/I_{c0}$  were also observed on the samples with stainless steel substrate both copper stabilized and brass laminated too.

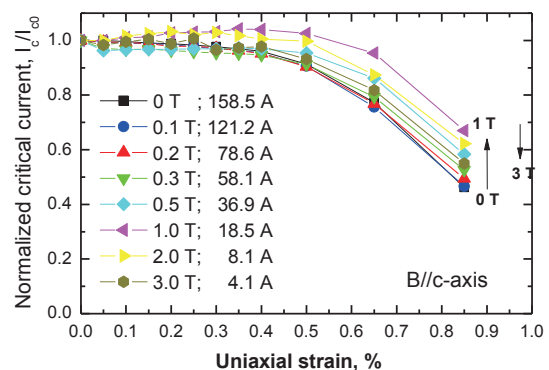


Fig. 2 Strain response of  $I_c/I_{c0}$  under magnetic field of brass laminated CC tape with Hastelloy substrate.

As a summary, it was observed that electromechanical property of CC tape strongly depends on the magnetic field especially when the field is directed perpendicular to the sample surface.

### References

- [1] H. S. Shin, M. J. Dedicataria, S. Awaji, K. Watanabe, *IEEE Trans. Appl. Supercond.* **22** 6600404 (2012).
- [2] D. C. van der Laan, J. W. Ekin, J. F. Douglas, C. C. Clickner, T. C. Stauffer, and L. F. Goodrich, *Supercond. Sci. Technol.* **23** 072001 (2010).

Keywords: superconducting, coating, mechanical properties,  
H.-S. Shin, M. J. Dedicataria, A. Gorospe (Andong National University), S. Awaji, H. Oguro ((MR, Tohoku University)  
E-mail: [hssin@andong.ac.kr](mailto:hssin@andong.ac.kr), [awaji@imr.tohoku.ac.jp](mailto:awaji@imr.tohoku.ac.jp)  
<http://www.hflsm.imr.tohoku.ac.jp/index.html>

## High-field magnetization and antiferromagnetic resonance in novel frustrated magnetic materials

Using high-field magnetization and antiferromagnetic resonance measurements we investigated two novel frustrated magnetic compounds,  $\beta$ -TeVO<sub>4</sub> and Cu<sub>2</sub>OCl<sub>2</sub>. In  $\beta$ -TeVO<sub>4</sub>, at 1.5 K, a clear field-induced transition is found at 5 and 10 T when field is in the *ab* plane and along *c*, respectively. On the other hand, field dependences of antiferromagnetic resonance imply a zero-field gap of ~150 GHz and ~300 GHz. In Cu<sub>2</sub>OCl<sub>2</sub>, we found no field induced transitions, while a zero-field gap is very clear and amounts ~100 GHz.

Frustrated magnetic systems, i.e., systems with competing magnetic interactions, often exhibit complex magnetic ground states, which are very sensitive to external perturbations. This effect becomes even more pronounced in low-dimensional systems and may lead to fascinating new phenomena, e.g. magnetoelectric coupling, and rich magnetic phase diagrams.

To pursue such intriguing effects, we undertook high-magnetic-field study of two novel magnetic compounds,  $\beta$ -TeVO<sub>4</sub> and Cu<sub>2</sub>OCl<sub>2</sub>, respectively. The former is a chain compound with dominant exchange interaction  $J \sim 21.4$  K and potentially significant competing next-nearest exchange interactions [1]. The latter, however, has a highly frustrated pyrochlore lattice with the exchange constant estimated to  $J \sim 110$  K [2]. At low temperatures,  $\beta$ -TeVO<sub>4</sub> exhibits three consecutive magnetic phases transitions, at 4.65, 3.28 and 2.28 K, which according to the neutron diffraction most likely correspond to three incommensurate magnetic phases. On the other hand, magnetic ordering temperature in Cu<sub>2</sub>OCl<sub>2</sub> is  $T \sim 70$  K, while the ground state is still unknown.

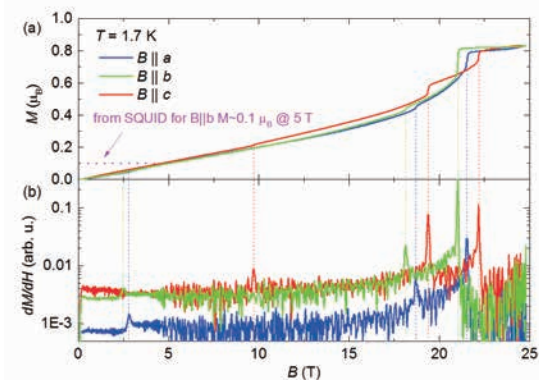


Fig. 1 Magnetization and its derivative in  $\beta$ -TeVO<sub>4</sub>.

Our results for  $\beta$ -TeVO<sub>4</sub> reveal that at 1.5 K, a field induced transition occurs that strongly depends on the field direction, i.e., when field is in the *ab* plane the transition is found at 5 T, while for the perpendicular orientation it occurs at 10 T. Further, we found at least two magnetic excitation branches with zero-field gaps of ~150 and ~300 GHz, which dramatically change in the high-field phase.

In Cu<sub>2</sub>OCl<sub>2</sub> the antiferromagnetic resonance at 1.5 K, i.e., well below magnetic transition, has a broad powder-like (box-shaped) spectrum. The broad feature extends for 3 to 8 T, at low and high frequencies, respectively. The spectral feature is touching the ordinate axis (0 T) at ~100 GHz, and hereby reveal the size of the zero-field gap in the excitation spectrum. With increasing frequency, a linear shift to higher frequencies is found, as typically encountered in antiferromagnetic systems.

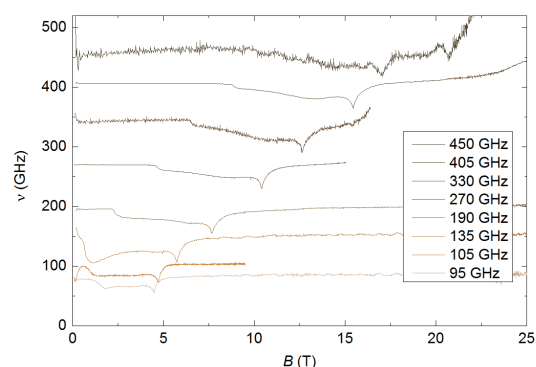


Fig. 2 Antiferromagnetic resonance in Cu<sub>2</sub>OCl<sub>2</sub>.

### References

- [1] Y. Savina et al., Phys. Rev. B 84, 104447 (2011).
- [2] M. Nishiyama et al., J. Phys.: Conference Series 320 012030 (2011).

Keywords: high magnetic field, electron spin resonance, magnetic properties  
 Matej Pregelj (Jožef Stefan Institute, Jamova c. 39, SI-1000 Ljubljana, Slovenia )  
 E-mail: matej.pregelj@ijs.si  
<http://www-f5.ijs.si/>

## Title- Single Visit Research Subject. Development of transparent ceramics superior to single crystal for high power laser application

Introductory part- I have continued on February 11-March 3, 2013 my fruitful cooperation with Pr. Yoshikawa and Pr. Goto Labs on Nd<sup>3+</sup>-doped Lu<sub>2</sub>O<sub>3</sub> ceramics made by SPS method. I also have attended ELYT Workshop 2013 at Zao Mountains and visited Dr. A. Ikesue inside the Japan Fine Ceramics Center of Nagoya.

After my recent stay at ICC-IMR on November-December 2012, I got again the great privilege to be helped by ICC-IMR to continue my fruitful cooperation at the Tohoku University between February 11 and March 3.

The first objective of my stay at IMR has been to show to Prof. Yoshikawa and Prof. Goto our new results of the spectroscopic measurements on Nd<sup>3+</sup>:Lu<sub>2</sub>O<sub>3</sub> transparent laser ceramics obtained for the first time by the non-conventional spark plasma sintering (SPS) method [1]. Absorption spectra have been analyzed at room temperature and at 4K at the Faculty of Chemistry of Wroclaw (Poland) by Dr.M. Guzik. Especially at 4K this fine spectroscopy shows not only Nd<sup>3+</sup> C<sub>2</sub> usual isolated ions but also the signatures of C<sub>2</sub>-C<sub>2</sub> and C<sub>2</sub>-C<sub>3i</sub> Nd<sup>3+</sup> pairs and even of the weak populated C<sub>3i</sub> isolated sites. Emission spectra of the expected laser lines <sup>4</sup>F<sub>3/2</sub> → <sup>4</sup>I<sub>11/2</sub>, at both 1076.4 nm and 1080.5 nm and concentration dependence of the <sup>4</sup>F<sub>3/2</sub> decays have also been analyzed at Lyon. The most striking feature is a strong concentration quenching seen in Fig.1 above 0.1% Nd<sup>3+</sup>, a weak value for laser material, so that laser output will need a sharp optimization to be pointed out.

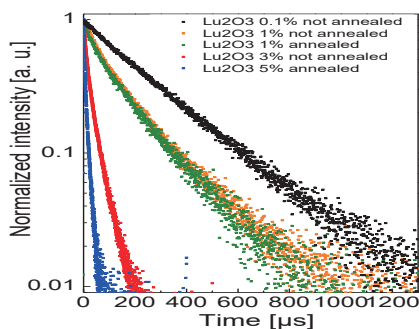


Fig.1 Decays of the Nd<sup>3+</sup> <sup>4</sup>F<sub>3/2</sub> meta-stable level at room temperature for several Nd<sup>3+</sup> concentrations.

At last, we use these samples to bring more knowledge on Nd<sup>3+</sup> isolated and pair sites by application of the site selective laser spectroscopy technique not only on Nd<sup>3+</sup> C<sub>2</sub> populated sites but also on less populated C<sub>3i</sub> inversion sites. In addition we have detected

Nd<sup>3+</sup> C<sub>2</sub>-Nd<sup>3+</sup> C<sub>2</sub> and Nd<sup>3+</sup> C<sub>2</sub>-Nd<sup>3+</sup> C<sub>3i</sub> pairs, respectively.

During this stay Dr. A. Ito has measured the values of the thermal conductivity, Dr. T. Ito and Prof. Kikuchi have started to register the TEM-EDX photos for the evaluation of Nd<sup>3+</sup> segregation in grains and grain boundaries.

It was also a great opportunity to attend the successful ELYT Workshop 2013 at hotel Laforet Zao To-o-gatta, February 17-20, 2013, organized by the new Associated International Laboratory (LIA in French) of "Engineering Science Lyon-Tohoku Laboratory", ELYT Lab. for the period 2013-2018. My oral communication gave the objectives of our project ELYT lab, M12- LASMAT, on "Rare earth-doped transparent laser ceramics by SPS method".

Then, I have visited the Laboratory of Dr. Akio Ikesue, World-Labo Co, Ltd, inside Japan Fine Ceramics Center in Nagoya on 24-26 February. Dr. Akio Ikesue also works on Nd<sup>3+</sup>:Lu<sub>2</sub>O<sub>3</sub> and Nd<sup>3+</sup>:Y<sub>2</sub>O<sub>3</sub> ceramics but made by conventional methods and has proposed me these samples to compare with ours obtained by SPS method.

At last, we have submitted two abstracts for SCINT2013 and REMAT2013 International Conferences [2-3].

### References

- [1] L. An, A. Ito, T. Goto, J. Amer. Cer. Soc. 94 (2011) 695-698 and 31(9) (2011) 1597-1602
- [2] Shunsuke Kurosawa, Akihiro Yamaji, Akira Suzuki, Yuui Yokota, Kenji Shirasaki, Yamamura Tomoo, Akihiko Ito, Takashi Goto, Georges Boulon, Akira Yoshikawa-Scintillation Properties of Nd<sup>3+</sup>-doped Lu<sub>2</sub>O<sub>3</sub> Transparent Ceramic in the Infra-Red Region. 12<sup>th</sup> International Conference on Inorganic Scintillators and their Applications (SCINT 2013). April 15-19, 2013, Shanghai (China)
- [3] G. Boulon, G. Alombert-Guget, Y. Guyot, A. Brenier, M. Guzik, T. Goto, A. Yoshikawa Nd<sup>3+</sup>-Doped Lu<sub>2</sub>O<sub>3</sub> transparent ceramic elaborated by Spark Plasma Sintering method: spectroscopic and structural characterizations. Invited paper at the 3<sup>rd</sup> International Conference on Rare earth Materials (REMAT 2013). April 26-28, 2013, Wroclaw (Poland).

Keywords: Ceramic, optical properties, laser,

Full Name: Georges Boulon, Institute Light Matter(ILM), UCBLyon1-CNRS

E-mail: georges.boulon@univ-lyon1.fr

http://georges-boulon.univ-lyon1.fr and http://ilm.univ-lyon1.fr

## Embrittlement trend curve (ETC) prediction of reactor pressure vessel (RPV) steels

A type of unstable radiation-induced defect in RPV steels, which a key to understanding neutron flux effects, has been characterized by positron annihilation and hardness measurements including recovery anneal. The defect structure involves mono-vacancy equivalent open volume and the formation is accelerated with flux. Flux compensated hardening trend curves suggested severer embrittlement than current prediction model after a long-term operation.

Unstable matrix damage (UMD) is a type of defect formed in aged displacement cascades, that anneals out continuously during reactor operation [1]. UMDs build up at high neutron flux in test reactor irradiations, confounding the results in two opposite ways – adding hardening and delaying formation of more typical hardening sources in power reactor conditions. The delay is due to point defect recombination enhanced at higher flux including at UMD sites[1]. Utilizing test reactor data to predict RPV long-term embrittlement trend curve (ETC) requires properly accounting for these effects. Hence, the objective of this study is to clarify the character and behavior of UMD, as well as to develop models of long-term predictions of radiation embrittlement after the flux effect compensation.

Positron annihilation spectroscopy (PAS) and hardness measurements before and after UMD recovery anneal at 350 °C for 5 h have been performed on 5 model RPV steels with systematic chemistry variation, irradiated in BR2 test reactor to two neutron dose levels; 1 and 2.5 x 10<sup>20</sup> n/cm<sup>2</sup> at 2 x 10<sup>13</sup> n/cm<sup>2</sup>s flux at 290 °C. PAS was also performed on the same set of alloys irradiated at other 10<sup>12</sup> and 10<sup>14</sup> n/cm<sup>2</sup>s flux conditions. Hardening database combined with other studies was analyzed and compared with current ETC models.

Specimens irradiated at 2 x 10<sup>13</sup> n/cm<sup>2</sup>s or higher flux showed significantly larger low momentum component Fraction (LMCF) in PAS as well as longer average positron lifetime than at 10<sup>12</sup> n/cm<sup>2</sup>s. Both measures of vacancy type damage increase with dose and flux, but recovery anneals reduce them to the level for irradiations at 10<sup>12</sup> n/cm<sup>2</sup>s condition. The second lifetime component reaches ≈ 180 ps at high dose. These PAS results suggest that UMD contains mono-vacancy size open volume defects that build up at least up to mid 10<sup>20</sup> n/cm<sup>2</sup> at a flux levels of the order of 10<sup>13</sup> n/cm<sup>2</sup>s or higher. The average UMD size may increase

with dose. Hardness recovery also increases with dose, but is significantly smaller at 2x10<sup>13</sup> than at 10<sup>14</sup> n/cm<sup>2</sup>s suggesting large flux dependence in the UMD number density. These new findings are to be considered in updating UMD models.

We obtain low flux long-time hardening estimates of the RPV steels by annealing out UMD and using effective dose after compensating for enhanced recombination at higher flux. Figure 1 shows an example for a Cu-free steel. It also shows that the current ETC models significantly under-predict the highest dose data in recent UCSB study (blue open diamond)[2]. The study confirmed the extra hardening is due to the formation of Mn-Ni-Si precipitates (so called late blooming phases, LBP), that were not observed at lower doses, but have long been predicted. This study clearly indicates that LBP hardening (dashed line) starts ≈ 5x10<sup>19</sup> n/cm<sup>2</sup>, typically ≈ 40 years of reactor operation, suggesting critical importance of ETC improvement. Further microstructural studies using atom-probe tomography and small angle neutron scattering are planned for future collaboration.

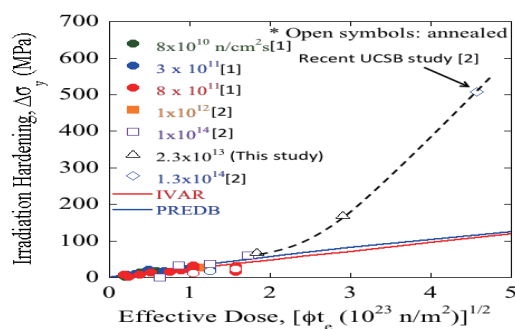


Figure 1 Irradiation hardening trend in a Cu free RPV steel.

### References

- [1] G.R.Odette, T.Yamamoto and D.Klingesmith, *Phil. Mag.*, vol. 85 pp.779-797 (2005)
- [2] P.Wells, T.Yamamoto, G.R.Odette et al., to be published

Keywords: nuclear materials, radiation effects, positron annihilation

Takuya Yamamoto (Univ. California Santa Barbara)

Collaborators: Peter Wells, G. Robert Odette (UCSB), Takeshi Toyama, Yasuyoshi Nagai (Tohoku U.)

E-mail: yamataku@engineering.ucsb.edu

## Synthesis of novel complex hydrides with mixed non-metal-based and metal-based complex anions

A dehydrating reaction of  $\text{LiBH}_4$  is drastically promoted by combining with  $\text{Mg}_2\text{FeH}_6$ . The dehydrating reaction of pure  $\text{LiBH}_4$  starts at approximately 650 K, which decreases with increasing the amount of  $\text{Mg}_2\text{FeH}_6$  added. The lattice parameter of  $\text{Mg}_2\text{FeH}_6$  measured by *in-situ* high-resolution synchrotron diffraction measurements suggests the possibility of forming a solid solution  $\text{Li}_{1-x}\text{Mg}_{2x}(\text{BH}_4)_{1-x}(\text{FeH}_6)_x$  with mixed non-metal-based  $[\text{BH}_4]^-$  and metal-based  $[\text{FeH}_4]^{4-}$  complex anions.

A complex hydride  $\text{LiBH}_4$ , consisting of  $\text{Li}^+$  cations and  $[\text{BH}_4]^-$  complex anions, is one of the promising materials for hydrogen storage due to its high hydrogen densities. The dehydrating temperature of above 673 K, however, is higher than the required temperature for solid state hydrogen storage materials, therefore many approaches have been made to improve the property [1].

We have found that the dehydrating temperature of  $\text{LiBH}_4$  can be lowered by combining with another complex hydride  $\text{Mg}_2\text{FeH}_6$  composed of  $\text{Mg}^{2+}$  and  $[\text{FeH}_4]^{4-}$  complex anions [2]. Fig. 1 shows the thermogravimetry/mass spectroscopy (TG-MS) profiles of  $(1-x)\text{LiBH}_4+x\text{Mg}_2\text{FeH}_6$  together with that of pure  $\text{LiBH}_4$ . The dehydrating reaction of pure  $\text{LiBH}_4$  starts at approximately 650 K by the following reaction:  $\text{LiBH}_4 \rightarrow \text{LiH} + \text{B} + 3/2\text{H}_2$ . The dehydrating temperature obviously decreases with increasing the amount of  $\text{Mg}_2\text{FeH}_6$  added. At  $x = 0.9$ , the hydrogen is released in the temperature range 530–580 K, which is more than 100 K lower as compared to pure  $\text{LiBH}_4$ .

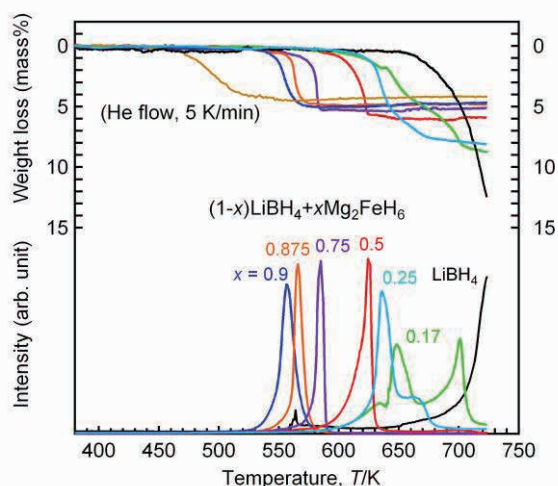


Fig. 1 TG-MS profiles of  $(1-x)\text{LiBH}_4+x\text{Mg}_2\text{FeH}_6$ .

The *in-situ* high-resolution synchrotron diffraction (SR-XRD) measurements, conducted at the Swiss-Norwegian Beam Line at the European Synchrotron Radiation Facility in Grenoble, suggest the possibility of forming a solid solution between  $\text{LiBH}_4$  and  $\text{Mg}_2\text{FeH}_6$ . As shown in Fig. 2, the lattice expansion of  $\text{Mg}_2\text{FeH}_6$  in  $\text{LiBH}_4+\text{Mg}_2\text{FeH}_6$  ( $x = 0.5$ ) differs from pure  $\text{Mg}_2\text{FeH}_6$  across the whole temperature range presumably due to the different thermal expansion coefficients. These results imply the possible solid solution formation via the following reaction:

$$(1-x)\text{LiBH}_4+x\text{Mg}_2\text{FeH}_6 \rightarrow \text{Li}_{1-x}\text{Mg}_{2x}(\text{BH}_4)_{1-x}(\text{FeH}_6)_x$$

Such a complex hydride with mixed non-metal-based and metal-based complex anions has not been reported to date although combinations of metal-based complex anions have been known to exist as the  $\text{Mg}_2\text{FeH}_6\text{-Mg}_2\text{CoH}_5$  system [3].

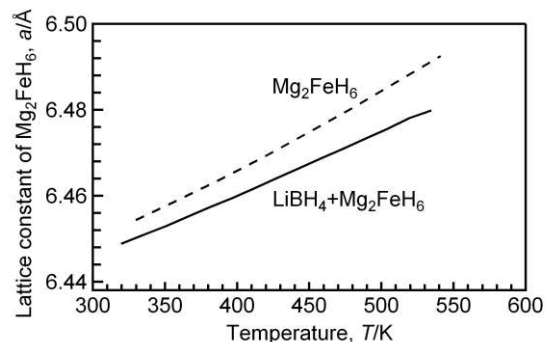


Fig. 2 Lattice expansions of  $\text{Mg}_2\text{FeH}_6$  in  $\text{LiBH}_4+\text{Mg}_2\text{FeH}_6$  ( $x = 0.5$ ) and pure  $\text{Mg}_2\text{FeH}_6$  obtained from *in-situ* SR-XRD profiles

### References

- [1] S. Orimo, Y. Nakamori, J.R. Eliseo, A. Züttel and C.M. Jensen, *Chem. Rev.* 107, 4111 (2007)
- [2] G. Li, M. Matsuo, S. Deledda, R. Sato, B.C. Hauback and S. Orimo, *Mater. Trans.* (in press)
- [3] S. Deledda and B.C. Hauback: *Nanotech.* 20, 204010 (2009)

Keywords: thermogravimetric analysis, x-ray diffraction, reactive ball milling  
 Motoki Matsuo (Hydrogen Functional Materials Division)  
 E-mail: mmatsuo@imr.tohoku.ac.jp  
<http://www.hydrogen.imr.tohoku.ac.jp/>





Activity Report

# Young Researcher Fellowships



## FY 2012 Young Researcher Fellowships

No.	Name	Host	Proposed Research	Title	Affiliation	Term
12FS1	Matthias Benjamin Jungfleisch	E. Saitoh	Spin Caloric Transport Phenomena and Spin Hall Effect Studies	Ph. D. Student	Technische Universität Kaiserslautern, Germany	2012.4-6
12FS2	Arnold Everhardt	E. Saitoh	Measurement of the Spin Seebeck effect in an insulating ferromagnetic Inorganic-Organic Hybrid	Master Student	University of Groningen, The Netherlands	2012.5-6
12FS3	Soo-Hyun Joo	H. Kato	Improving the Ductility and Wear Property of Bulk Metallic Glasses Using High Pressure Torsion	Ph. D. Student	Pohang Univ of Science and Technology	2012.6-7

## Heat-induced damping manipulation in YIG/Pt heterostructures

The damping of magnetization in a magnet was manipulated by heat-induced spin-transfer torque. In the yttrium iron garnet/platinum (YIG/Pt) heterostructure the magnetization relaxation, detected by spin pumping method, was controlled by a temperature gradient applied across thickness.

In the field of magnon spintronics the control and manipulation of magnetization relaxation are gaining much attention. Here, we show the manipulation of spin-wave damping utilizing a temperature difference across the thickness of an yttrium iron garnet (YIG)/platinum (Pt) multi-structure (Fig. 1(a)). It has been demonstrated that this temperature difference  $\Delta T$  gives rise to the longitudinal spin Seebeck effect[1]: an imbalance between the effective magnon and the effective electron temperatures causes a spin current across the YIG/Pt interface. In addition to this effect, since the created spin current transfers spin angular momentum, a torque is exerted on the magnetization (Fig. 1(b)), and damping modulation in the magnetization is expected to be detected by spin pumping method.

In the experiment an external magnetic field  $H$  is applied perpendicularly to the YIG waveguide in the YIG film plane (Fig. 1(a)). The magnetization precession is driven by the alternating microwave field of a continuous microwave signal. The spin currents injected into Pt film by spin pumping is detected as an electric voltage by the inverse spin Hall effect (ISHE). The temperature gradient applied across thickness was monitored by an infrared (IR) camera. Although in the magnetic resonance condition the sample temperature rises producing an additional electric voltage due to spin Seebeck effect, this can be subtracted by monitoring the sample temperature using the IR camera.

In Fig. 1(c) the ferromagnetic resonance linewidth  $\Delta H_{\text{FMR}}$  were shown as a function of applied temperature gradient  $\Delta T$  and microwave powers of +14 dBm, +20 dBm, and +25 dBm at 4 GHz. The magnetization precession is either enhanced or suppressed depending on the sign of  $\Delta T$ . As it is visible from Fig. 1(c), the variation of the linewidth per 1 degree temperature difference (slope in Fig. 1(c)) is approximately the same for all microwave powers.

Assuming that the observed heat-induced damping variation is due to an effective spin current representing thermally induced torque, we calculate the variation of the magnetization relaxation in YIG/Pt hetero-structures based on the model developed in Ref. 3. We modify this model by substituting a heat-induced spin current for a SHE-generated spin current: the charge current  $J_c$  is replaced by the temperature difference  $\Delta T$ . Then the spin transfer due to the temperature difference across the YIG/Pt interface has been estimated comparing to previous works that use SHE-generated spin currents. It turns out that the heat-induced spin current density  $J_s$  per degree is of the order  $10^9 \text{ A/m}^2$ .

In conclusion, we performed detection of damping modulation by heat-induced spin transfer torque in magnetic materials introducing analysis for the calculation of the heat-induced spin current density.

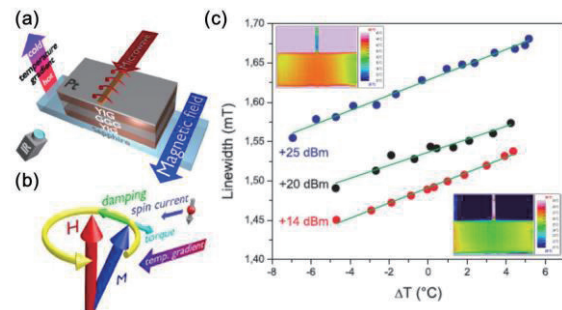


Fig. 1 (a) Experimental setup of the heat-induced damping manipulation in the Pt/YIG. (b) Schematic of spin-transfer torque damping modulation. (c) Line-width of the ferromagnetic resonance as a function of temperature gradient.

### References

- [1] K. Uchida *et al.*, Nature Mater. 9, 894 (2010)
- [2] M. B. Jungfleisch *et al.*, Appl. Phys. Lett. 102, 062417 (2013)
- [3] K. Ando, *et al.*, Phys. Rev. Lett. 101, 036601 (2008)

Keywords: spin current, spin transfer, ferromagnetic  
Eiji Saitoh (Materials Property Division)  
E-mail: eizi@imr.tohoku.ac.jp  
<http://saitoh.imr.tohoku.ac.jp/>

## Measurement of the Spin Seebeck Effect in an Insulating Ferromagnetic Inorganic-Organic Hybrid

The Spin Seebeck effect is a newly discovered effect which can convert a heat flow into a spin voltage in insulators [1]. An attached Pt film in the longitudinal configuration can then transform it into an electrical voltage [2]. So far, the spin Seebeck has only been found in ferromagnetic inorganic materials, while this work tries to extend it to ferromagnetic inorganic-organic hybrids [3].

The inorganic-organic hybrid under study is a two-dimensional ferromagnet with a (finite) Curie temperature of 13K [3]. The structure is shown in Fig. 1(a).

A new setup for the measurement of the spin Seebeck effect in this material was made, based on the longitudinal spin Seebeck setup published before [2]. Since the Curie temperature is too low for the measurement setup used in those studies, the new setup was made for a Quantum Design Physical Property Measurement System (PPMS) which can reach lower temperatures. The sample is clamped between a copper heat sink and a sapphire plate which is heated during the experiment, with temperature sensors on both sides. A temperature gradient is created over the sample, which creates an electrical voltage by the spin Seebeck effect and the inverse spin Hall effect in the Pt layer sputtered on top of the material.

The new setup was first tested for a material of which the spin Seebeck signal is known from other setups: Yttrium Iron Garnet (YIG). This measurement is shown in Fig. 1(b) where it can be seen that the signal is magnetic field dependent which is the key characteristic of a spin Seebeck signal. Other features are also equal to the signals reported by earlier studies [2]. So it has been found that this new setup can find spin Seebeck signals which also proves the robustness of this effect.

The same experiments have been performed for the inorganic-organic hybrids with the result also shown in Fig. 1(b). No dependence of the voltage on the magnetic field could be found in this experiment. The noise in this experiment, while lower than in the previous setup, was still higher than the expected magnitude of the spin Seebeck effect in this material in this

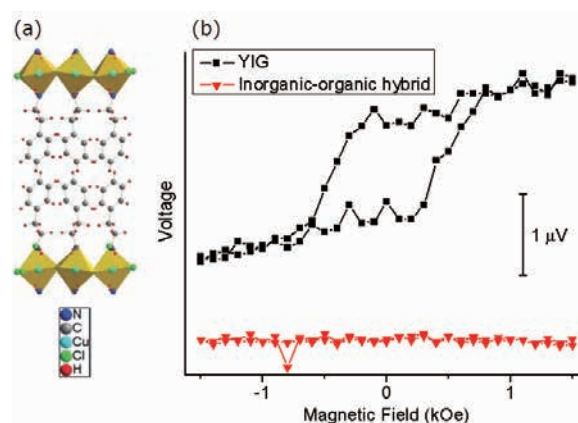


Fig. 1 (a) Structure of the inorganic-organic hybrid. (b) Dependence of the voltage in the spin Seebeck experiment on the magnetic field for both the reference material YIG as the inorganic-organic hybrid at 10 K.

measurement. Tackling problems of this noise level and the formation of cracks in the sample material are expected to be very difficult to solve. It seems wiser to explore other materials to measure spin Seebeck effects in (partly) organics.

Concluding, this study has created a new measurement setup for the measurement of the spin Seebeck effect which has reduced the noise level and proven the spin Seebeck effect of known materials in a different environment. The measurement of the spin Seebeck effect in inorganic-organic hybrids has proven to be a very difficult task and has not produced meaningful results.

### References

- [1] K. Uchida *et al.*, *Nature Mater.* 9, 894 (2010)
- [2] K. Uchida *et al.*, *Appl. Phys. Lett.* 97, 172505 (2010)
- [3] A. O. Polyakov *et al.*, *Chem. Mater.* 24, 133 (2012)

Keywords: spin current, organic, ferromagnetic  
 Eiji Saitoh (Materials Property Division)  
 E-mail: eizi@imr.tohoku.ac.jp  
<http://saitoh.imr.tohoku.ac.jp/>

## The pressure and torsion effects of High Pressure Torsion process on Zr-based bulk metallic glasses

In this study, Zr-based bulk metallic glasses were deformed by high pressure torsion process at room temperature. After each stage in the HPT process, the structural and mechanical properties of the disk sample were observed to reveal pressure and shear strain effects. Nano-indentation creep tests proved there were significant changes of free volume and residual stress was analyzed by finite element method.

Bulk metallic glasses (BMGs) generally suffer from low ductility and catastrophic failure at low temperature. The discrete deformation in localized shear bands governs the deformation mechanism in metallic glasses. The shear band region is severely plastically deformed and there is a significant change of structure, such as the increase in free volume. High pressure torsion (HPT) has been the subject of many investigations as a new method of processing because of its ability to impose extremely high strain and hydrostatic pressure without failure [1]. It is reported that the HPT process introduces an excessive free volume and nanoscale microstructural heterogeneity in BMGs and enhances ductility of BMGs [2]. The HPT process can be divided into two stages. The first stage is compression stage and the second stage is torsional stage. It is important to know that effects of pressure and torsion are different in BMGs due to free volume mechanism.

Zr<sub>65</sub>Al<sub>7.5</sub>Ni<sub>10</sub>Cu<sub>12.5</sub>Pd<sub>5</sub> BMG was produced via arc melting the pure elements (99.99%) under a purified argon atmosphere in button-shape ingots of the desired composition. Each button-shape ingot was turned over and re-melted four times to ensure the homogeneity of the chemical composition. BMG cylindrical rods with a diameter of 8 mm were prepared via tilt casting into copper molds.

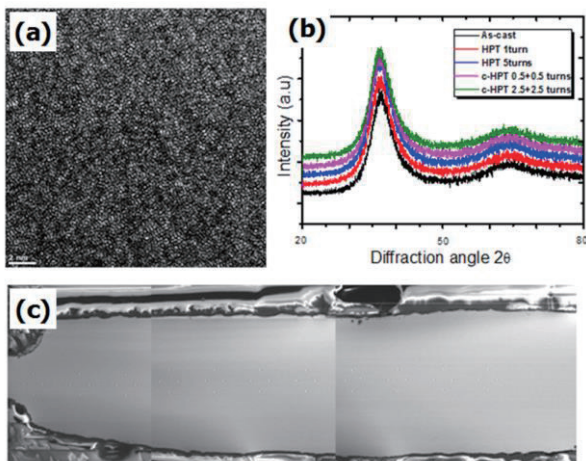


Fig.1 (a) High resolution TEM image after 5 turns, (b) XRD results and (c) SEM image on radial surface after 5 turns

Fig. 1 (a) and (b) show high resolution TEM and

XRD results of HPT processed bulk metallic glass, respectively. Amorphous state was maintained without nanocrystallization during the HPT process. In Fig. 1(c), it is noticeable the BMGs were severely deformed without failure.

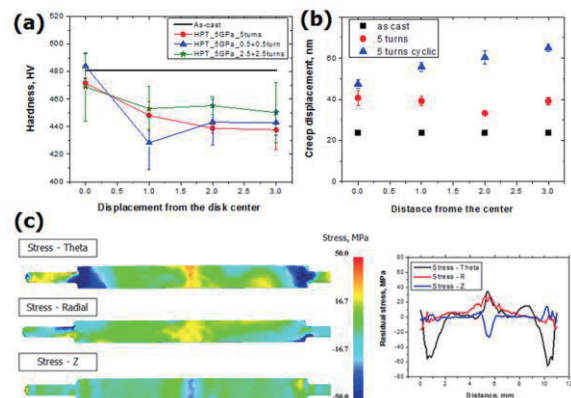


Fig. 2 (a) Hardness results, (b) Nano-indentation creep results and (c) Residual stress analysis using FEM

Hardness was increased compared to as-cast specimens after the compression stage (not shown here) due to free volume decrease under high pressure. Then, hardness was dramatically decreased along radial direction after the torsional stage (Fig. 2 (a)). In shear bands region, structurally free volume is higher than undeformed matrix. The HPT process gives more shear strain from the center to edge, so, lower hardness was observed at the edge. BMGs show creep displacement at the ambient temperature, and the amount of creep is dependent on load and free volume. Fig. 2 (c) shows larger creep displacement after HPT process. From the NI tests, it is concluded that the shear strain effect is stronger than pressure even at the center. Compressive residual stress can interrupt shear band propagation and enhance ductility of BMGs. Residual stress after HPT process was analyzed by finite element method (Fig. 2(c)).

### References

- [1] A.P. Zhilyaev and T.G. Langdon, Prog. Mater. Sci. 53(6), 893 (2008)
- [2] Y.B. Wang, D.D. Qu, X.H. Wang, Y. Cao, X.Z. Liao, M. Kawasaki, S.P. Ringer, Z.W. Shan, T.G. Langdon and J. Shen, Acta Mater. 60, 253 (2012)

Keywords: metallic glass, deformation, nano-indentation  
Soo-Hyun, Joo (Pohang University of Science and Technology)  
E-mail: jjsh83@postech.ac.kr  
http://snmpl.postech.ac.kr



---

---

## ICC-IMR FY2012 Activity Report

---

Edited by ICC-IMR Office  
Published in February, 2018

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

Printing: HOKUTO Corporation

