REIMEI International workshop: **Physics of Advanced Functional Materials**

From 10th Oct.(Thu) to 11th Oct.(Fri) 2024

Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan

10.10.2024 (Thursday)

09:30	Reception	
09:50	Opening J. Ieda (JAEA)	
10:00	Talk1	O. Klein (CEA Grenoble/UGA)
10:30	Talk2	T. Seki (Tohoku U)
11:00	Talk3	J. Chen (SUSTech)
11:30	Lunch (2H)	
13:30	Talk4	K. Oyanagi (Iwate U)
14:00	Talk5	T. Kikkawa (JAEA)
14:30	Talk6	Y. Araki (JAEA)
15:00	Break	
15:30	Talk7	M. Ohta (Shimane U/ PROTERIAL)
16:00	Talk8	F. Kammerbauer (JGU Mainz)
16:30	Talk9	J. Barker (U Leeds)
17:00	P. Fulde Memorial Session	
19:00	Banquet @Another Space (Access: http://www.another-space.jp/shop)	

11.10.2024 (Friday)

9:30	Reception	
10:00	Talk10	G. E. W. Bauer (UCAS, Tohoku U)
10:30	Talk11	N. Ikeda (Okayama U)
11:00	Talk12	M. Matsuura (CROSS)
11:30	Lunch (2H)	
13:30	Talk13	I. Lobzenko (JAEA)
14:00	Talk14	M. Enoki (Shimane U)
14:30	Talk15	Y. Ikeda (Tohoku U)
15:00	Break	
15:30	Talk16	S. Tsutsui (JASRI)
16:00	Talk17	K. Z. Suzuki (JAEA)
16:30	Talk18	H. Isshiki (JAEA)
17:00	Closing	K. Takanashi (JAEA)

Orbital Angular Momentum of Azimuthal Spin-Waves

T. Valet,[1] K. Yamamoto,[2] B. Pigeau,[3] G. de Loubens,[4] and O. Klein[1,†]

[1]Université Grenoble Alpes, CEA, CNRS, Grenoble INP, Spintec, 38054 Grenoble, France
[2]ASRC, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan
[3]Université Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, Grenoble, France
[4]SPEC, CEA, CNRS, Université Paris-Saclay, 91191 Gif-sur-Yvette, France
*E-mail: oklein@cea.fr

In the context of a growing interdisciplinary interest in the angular momentum of wave fields, that of spin waves has yet to be fully explored, with the extensively studied notion of spin transport being only part of the story. Here we report experimental evidence for magnon orbital angular momentum by observing the lifted degeneracy of waves with counter-rotating wave fronts [1]. This requires an unambiguous formulation of spin and orbital angular momenta for spin waves, which we provide in full generality based on a systematic application of quantum field theory techniques. The results unequivocally establish magnetic dipole-dipole interactions as a magnetic-field controllable spin-orbit interaction for magnons (see Fig.1). Our findings open a new research direction exploiting the spectroscopic readability of angular momentum for azimuthal spin waves and beyond.

This work is partially supported by REIMEI research program from Japan Atomic Energy Agency.

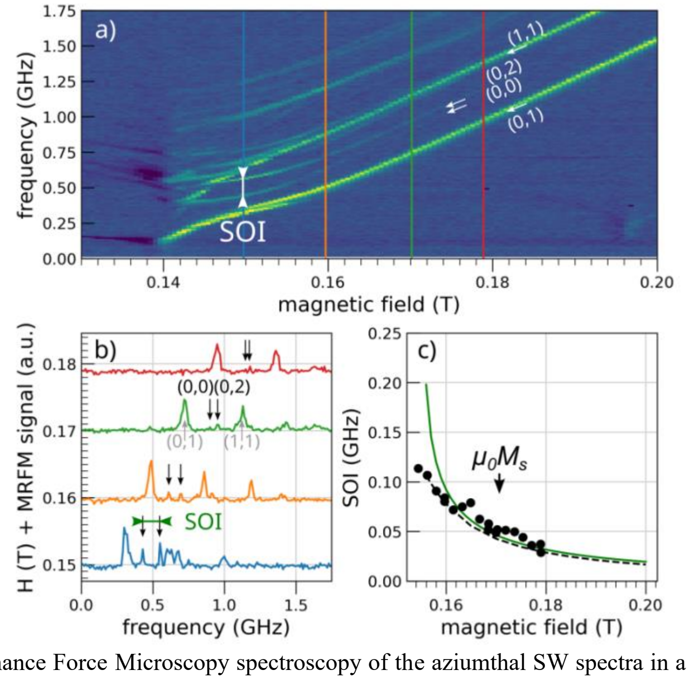

Fig.1 : (a) Magnetic Resonance Force Microscopy spectroscopy of the aziumthal SW spectra in a normally magnetized 1µm diameter YIG disk. (b) The spin-orbit interaction (SOI) is measured from the frequency split between (0,2) and (0,0) modes which have opposite orbital index n_L=±1. (c) Magnetic field dependence of the SOI. The dots are the experimental points, the solid line is the analytical prediction and the dashed line is the result of the micromagnetic simulation, assuming a misalignment of ~0.5° between the applied magnetic field and the normal of the disk.

[1] T. Valet et al. «Orbital Angular Momentum of Azimuthal Spin-Waves» to appear on arXiv

Control of Magneto-Elasticity in Magnetic Thin Films

T. Seki[1,2*], and K. Ito[1]

[1] Institute for Materials Research, Tohoku University, Sendai, Japan
[2] Center for Science and Innovation in Spintronics, Tohoku University, Sendai, Japan
*E-mail: takeshi.seki@tohoku.ac.jp

Flexible spintronics has opened new avenue to promising devices and applications in the field of wearable electronics. Particularly, miniaturized strain sensors exploiting the spintronic function have attracted considerable attention, in which the magnetoelasticity linking magnetism and lattice distortion is a vital property for high-sensitive detection of strain.
In this talk, we will introduce our recent research activity for controlling the magneto-elastic properties of the magnetic thin film. First, we share the topics of the magnetostriction for Fe-Ga epitaxial thin films grown on the different substrates [1]. Fe-Ga is one of the representative materials exhibiting the large magnetostriction in the bulk form. We investigated the magnetostriction values for the Fe-Ga epitaxial thin films employing the optical cantilever method, and our results clearly indicated that large magnetostriction comparable to the bulk values can be achieved even in the thin film form. At the same time, it was confirmed that optical cantilever method we employed is reliable.
Then, we show the demonstration that the magnetoelastic properties of Fe_4N can be significantly varied by partially replacing Fe with Co or Mn. The high quality Fe_4N film exhibits large negative magnetostriction along the [100] direction (λ_{100}) of -121 ppm while $Fe_{3.2}Co_{0.8}N$ shows λ_{100} of +46 ppm. This wide-range tunability of λ_{100} from -121 to +46 across 0 allows us to thoroughly examine the correlation between the magnetoelasticity and other magnetic properties. We experimentally find the strong correlation between λ_{100} and magnetic damping (α). The enhanced extrinsic term of α is attributable to the large two magnon scattering coming from the large magnetostriction. In addition to the systematic experiment, we carried out the first-principles calculation, which indicates that the density of states at the Fermi level plays a primal role to determine both λ_{100} and the intrinsic term of α. Thanks to the giant tunability and the bipolarity of magnetoelasticity, magnetic nitrides are candidate materials for high-sensitive spintronic strain sensors [2].

The studies shown here were done in collaboration with Prof. Yasushi Endo, Mr. Hao Ding, Prof. Koki Takanashi, Dr. Ivan Kurniawan, Dr. Yoshio Miura, and Prof. Yusuke Shimada.

References

[1] H. Ding, **TS** *et al.*, *J. Phys. D: Appl. Phys.* 57, 385002-1-10 (2024).
[2] K. Ito, **TS** *et al.*, arXiv: 2403.16679

Strong magnon-magnon coupling and unidirectional exchange spin waves in magnetic nanostructures

Jilei Chen

[1] Shenzhen Institute for Quantum Science and Engineering,
Southern University of Science and Technology, Shenzhen 518055, China

*E-mail: chenjl6@sustech.edu.cn

Magnons, the quanta of spin waves, are collective precessions of electron spins in magnetic materials, which do not involve charge motion during propagation, and thus can avoid Joule heating in information transmission, making them potential candidates for the next-generation of low-power electronic devices. In this talk, I will introduce the observation of strong interlayer magnon-magnon coupling in magnetic metal-insulator hybrid nanostructures. A large anticrossing gap up to 1.58 GHz is observed between the ferromagnetic resonance of the metallic nanowires and the in-plane standing spin waves of a low-damping yttrium iron garnet (YIG) film. Using this effect, we also experimentally observe the long-distance propagation of ultra-short-wavelength spin waves with wavelengths as low as 50 nm, and demonstrate the unidirectional behavior of such spin waves. A nanoscale magnonic interferometer can be designed based on the unidirectional spin waves. We also discuss the experimental observation of nonlocal three-magnon scattering between spatially separated magnetic systems. Above a certain threshold power, a CoFeB Kittel magnon splits into a pair of counter-propagating YIG magnons which can be detected by the inverse spin Hall effect. Our results demonstrate the nonlocal detection of two separately propagating magnons emerging from one common source that may enable quantum entanglement between distant magnons for quantum information applications.

Spin current generation in paramagnetic insulators

K. Oyanagi[1]*

[1] Faculty of Science and Engineering, Iwate University, Morioka 020-0051, Japan
*E-mail: k.0yanagi444@gmail.com

Up to now, the discoveries of new materials which show spintronic functions have stimulated progress in spintronics. After the demonstration of the injection/propagation/detection of spin currents in normal metal (NM)/ferrimagnetic insulator junctions [1], a magnetic ordering insulator becomes an important player in spintronics. In addition to the magnetically ordered insulators, paramagnetic insulators are found to appear as spintronics materials showing several spintronic functions such as spin pumping [2], spin Seebeck effects [3], long-range spin transport [4] and spin Hall magnetoresistance [5].

Here, we investigated the spin current generation in NM/paramagnetic insulator (PI) junctions. We modeled a general formula of the interface spin current at NM/PI based on a linear response approach and applied the model to explain the experimental observation of paramagnetic spin Seebeck effects in the Pt/$Gd_3Ga_5O_{12}$ junction. The comparison between the calculation and experiment reveals the role of the interfacial spin current in the paramagnetic spin Seebeck effect [6]. In addition, our new experimental results indicate the importance of bulk spin transports in the paramagnetic spin Seebeck effect.

This research is collaboration with Prof. Saitoh, Assis. Prof. T. Kikkawa, Dr. S. Takahashi.

[1] Y. Kajiwara K. Harii, S. Takahashi, J. Ohe, K. Uchida, M. Mizuguchi, H. Umezawa, H. Kawai, K. Ando, K. Takanashi, S. Maekawa, and E. Saitoh, "Transmission of electrical signals by spin-wave interconversion in a magnetic insulator," Nature **464**, 262-267 (2010).

[2] Y. Shiomi and E. Saitoh, "Paramagnetic spin pumping," Physical Reviwe Letters **113**, 266602 (2015).

[3] S. M. Wu, J. E. Pearson, and A. Bhattacharya, "Paramagnetic spin Seebeck effect," Physical Review Letters **114**, 186602 (2015).

[4] K. Oyanagi, S. Takahashi, L. J. Cornelissen, J. Shan, S. Daimon, T. Kikkawa, G. E. W. Bauer, B. J. van Wees, and E. Saitoh, " Spin transport in insulators without exchange stiffness," Nature Communications **10**, 4740 (2019).

[5] K. Oyanagi, J. M. Gomez-Perez, X.-P. Zhang, T. Kikkawa, Y. Chen, E. Sagasta, A. Chuvilin, L. E. Hueso, V. N. Golovach, F. S. Bergeret, F. Casanova, and E. Saitoh, "Paramagnetic spin Hall magnetoresistance," Physical Review B **104**, 134428 (2021).

[6] K. Oyanagi, S. Takahashi, T. Kikkawa, and E. Saitoh, "Mechanism of paramagnetic spin Seebeck effect," Physical Review B **107**, 014423 (2023).

Current-driven coupled nuclear- and electron-spin dynamics

Takashi Kikkawa[1,2*]

[1] Department of Applied Physics, The University of Tokyo, Tokyo, Japan
[2] Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan.
*E-mail: t.kikkawa@ap.t.u-tokyo.ac.jp

Nuclear spins, with their long coherence times, are fundamental to nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI), serving as powerful tools for probing microscopic properties of matter. In addition to having a spin angular-momentum comparable to that of electrons, nuclear spins have unique advantages. For instance, they can maintain high entropy even at extremely low temperatures and strong magnetic fields, where electron spin dynamics are inevitably frozen out. Despite these fascinating properties, the application of nuclear spins in spintronics has been limited. Recently, however, spin-current generation from nuclear spins have been reported [1,2]. These studies utilize an antiferromagnetic insulator $MnCO_3$, in which nuclear and electron spins are coupled by strong hyperfine interaction between them, showing the potential to harness hyperfine coupling for exploring nuclear spintronic phenomena. In this presentation, I will discuss our recent results on current-induced nuclear and electron spin dynamics in a metallic ferromagnet and their electrical detection through hyperfine interactions.

This work has been done in collaboration with J. Numata, T. Makiuchi, E. Saitoh (from University of Tokyo), T. Kubota, T. Seki, S. Takahashi (from Tohoku University), and H. Chudo, M. Umeda, K. Takanashi (from Japan Atomic Energy Agency).

[1] Y. Shiomi, J. Lustikova, S. Watanabe, D. Hirobe, S. Takahashi, and E. Saitoh, Spin pumping from nuclear spin waves, Nat. Phys. **15**, 22 (2019).

[2] T. Kikkawa, D. Reitz, H. Ito, T. Makiuchi, T. Sugimoto, K. Tsunekawa, S. Daimon, K. Oyanagi, R. Ramos, S. Takahashi, Y. Shiomi, Y. Tserkovnyak, and E. Saitoh, Observation of nuclear-spin Seebeck effect, Nat. Commun. **12**, 4356 (2021).

Inductance and capacitance emerging from topological electromagnetism

Yasufumi Araki
Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan.
*E-mail: araki.yasufumi@jaea.go.jp

Inductors and capacitors are the most essential elements in electronic circuits. They are used for filtering and amplification of electronic signals, which are indispensable in any contemporary electronic devices. The operation principles of commercially used inductors and capacitors are based on classical electromagnetism described by Maxwell's equations. Since they operate with conduction currents in metals, power loss by internal resistance is inevitable. Such a power loss prevents further integration of electronic circuits, which needs to be resolved for the development of information-oriented society.

In this presentation, we report our recent theoretical proposal of the novel inductors and capacitors using topological insulator (TI) heterostructures, with significantly improved power efficiency [1]. TIs show various anomalous responses between electricity and magnetism, such as the anomalous Hall effect and the spin-charge conversion, which are free from power loss by Joule heating. By combining such anomalous magnetoelectric responses with spin dynamics in magnets, we show the emergence of inductance and capacitance in heterostructures of TIs and magnets, with significantly reduced power loss. We build a unified theoretical framework to extract the inductance and capacitance, on the basis of topological quantum field theory [2] describing the anomalous magnetoelectric responses. From this theoretical framework, we numerically evaluate the inductance and capacitance in two-dimensional (2D) and three-dimensional (3D) heterostructures of TI and ferromagnetic insulator (FI). We also compare their power efficiency with the "emergent inductors" reported in previous studies [3-7], which use spin dynamics in metallic magnets to generate inductance, and show that TIs can highly reduce the power loss in inductors.

This research is collaboration with Dr. J. Ieda.

[1] Y. Araki and J. Ieda, J. Phys. Soc. Jpn. **92**, 074705 (2023) .
[2] X.-L. Qi, T. L. Hughes, and S.-C. Zhang, Phys. Rev. B **78**, 195424 (2008).
[3] N. Nagaosa, Jpn. J. Appl. Phys. **58**, 120909, (2019).
[4] J. Ieda and Y. Yamane, Phys. Rev. B **103**, L100402 (2021).
[5] Y. Yamane, S. Fukami, and J. Ieda, Phys. Rev. Lett. **128**, 147201 (2022).
[6] T. Yokouchi, F. Kagawa, M. Hirschberger, Y. Otani, N. Nagaosa, and Y. Tokura, Nature **586**, 232 (2020).
[7] A. Kitaori, N. Kanazawa, T. Yokouchi, F. Kagawa, N. Nagaosa, and Y. Tokura, Proc. Nat. Acad. Sci. **118**, e2105422118 (2021).

Observation of magnetic domains in Fe-based amorphous alloys using polarized neutron magnetic imaging

M. Ohta[1,3*], N. Ito[2], H. Hayashida[4], T. Shinohara[5], K. Hiroi[5]

[1]PRPTERIAL, Global Research & Innovative Technology Center, Kumagaya, Japan

[2]PRPTERIAL, Yasugi Works, Yasugi, Japan

[3]Shimane University, Next Generation Tatara Cocreation Center, Matsue, Japan

4CROSS, Tokai, Japan

[5]Japan Atomic Energy Agency, Tokai, Japan

*E-mail: motoki.ota.tw@riko.shimane-u.acjp

In commercially available Fe-based amorphous ribbons, so-called fish scales (FS), which are periodically shallow grooves spaced several millimeters apart, are formed on the surface of the ribbon in order to reduce iron loss. These FS are formed by controlling the casting conditions and vibrating the surface of the liquid metal as it solidifies. However, it has become clear that there is room for investigation into the iron loss reduction effect of FS[1]. Therefore, in order to verify the effectiveness of FS, the magnetic domain structure of Fe-based amorphous alloy ribbons with FS was confirmed three-dimensionally by polarized neutron magnetic imaging method. In samples with FS, refinement of magnetic domains has occurred, but the soft domain properties have not been significantly improved. The background to this is that there are few domain walls that can move smoothly even if domaines are refined and the effect on reducing excess eddy loss is limited. When we attempted to refine the magnetic domains by adding laser processing to a smooth surface ribbon with low FS, excessive eddy current loss was significantly suppressed. This effect persists not only in single sheet samples but also in wound cores. In the future, we plan to proceed with polarized neutron magnetic imaging to verify the effectiveness of laser processing..

[1] N. Ito, H, Itagaki, M. Ohta, *J. Magn. Magn. Mater.* 564 (2022) 170168

Effects of chiral polypeptides on magnetic domain pinning and skyrmion dynamics

F. Kammerbauer, Y. Kapon, Theo Balland, S. Yochelis, Y. Paltiel and M. Kläui

[1]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany
[2] Institute of Applied Physics, Faculty of Sciences, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

Chirality is an intrinsic property of many fascinating systems. Some of them are hosted in magnetic thin films, as chiral spin structures, such as skyrmions, others are within the vast world of chemistry, helix structures for example, most famously DNA. Chiral polypeptides are of specific interest within this world as they display large chiral-induced spin-selectivity (CISS), a property unique to chiral systems and also of recent interest to the magnetism community. CISS provides new methods to manipulate magnetic materials and it has recently be shown that the adhesion of chiral molecules can switch the magnetization of a thin Co layer [Ben Dor]

We investigate the interaction of chiral molecules with magnetic thin films utilizing magneto-optical Kerr-effect (Kerr) microscopy. We employ different methods to adhere the chiral polypeptides, such as drop-casting, self-assembly, and selective adhesion. We observe the effects of domain pinning, rotation of domains, the delay of the spin reorientation transition, and reduced thermal motion of the skyrmions. These results display the early results of incorporating CISS into magnetic thin films. Showcasing the potential of chiral molecules to address challenges in skyrmionics, with promising applications in advanced magnetic devices.

[1] O. Ben Dor et al. ‘Magnetization Switching in Ferromagnets by Adsorbed Chiral Molecules without Current or External Magnetic Field’. *Nature Communications* **8**, 14567 (2017)

Atomistic modelling of amorphous magnets

J. Barker[1*]

[1]School of Physics and Astronomy, University of Leeds, United Kingdom
*E-mail: j.barker@leeds.ac.uk

Amorphous magnetism was a popular topic of study in the 1970s. Nevertheless, amorphous magnets are still commonly used in experiments and applications, such as GdFeCo for magneto-optics and CoFeB for spintronics. Modelling of these materials is often done using random lattice models or homogeneous systems, ignoring the true local disorder. Here, I will present methods and results from our studies where we attempt to include the true atomic disorder.

We use reverse Monte Carlo methods to generate realistic amorphous structures based on experimental X-ray and neutron diffraction data. We then use a Heisenberg Hamiltonian with distance-dependent exchange interactions and solve the Landau-Lifshitz-Gilbert equation to study the dynamics and thermodynamics of these systems. In particular, we studied CoP [1], a material where past experiments suggested the possible existence of roton-like magnon excitations [2].

We calculated the inelastic neutron scattering cross-section from our non-lattice model and found a feature at the same location as the supposed roton dip (Fig. 1). Our conclusion, however, is that this feature is a remnant of short-range local order, rather than an exotic magnon excitation.

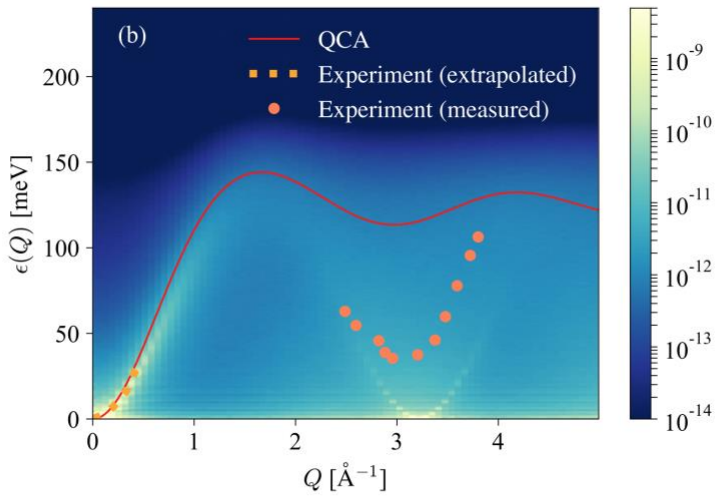

Fig.1: Calculated inelastic neutron scattering cross section of Co_4P compared with red: quasi-crystalline approximation (QCA) and orange: experimental inelastic neutron measurements of the 'roton-like' excitations.

[1] M. Kameda *et al.*, Magnon spectrum of the amorphous ferromagnet Co_4P from atomistic spin dynamics, Phys. Rev. B **106**, L060403 (2022)

[2] H.A. Mook *et al.*, Magnetic Excitations in the Amorphous Ferromagnet Co_4P, Phys. Rev. Lett. **34**, 1029 (1975)

Dipolar chirality of magnon transport in thin magnetic films

G.E.W. Bauer[1,2]

[1]AIMR, IMR & CSIS, Tohoku University, Sendai, Japan
[2]KITS-UCAS, Beijing, China
*E-mail: g.e.w.bauer@gmail.com

Non-reciprocity, chirality, or uni-directionality of transport are ubiquitous phenomena in condensed matter physics that are often ascribed to the relativistic spin-orbit interaction. However, in the case of magnon transport, the dipolar interaction is often a much stronger source of chiral magnon propagation [1,2]. In recent years, Yu Tao and collaborators established the nature of this chirality in thin magnetic films [3] and unveiled new observable consequences.

In this talk I will review this issue and discuss recent results.

[1] L.R. Walker, Magnetostatic modes in ferromagnetic resonance, Phys. Rev. **105**, 390 (1957); R.W. Damon, J.R. Eshbach, Magnetostatic modes of a ferromagnet slab, J. Phys. Chem. Solids **19** 308 (1961).

[2] K. Yamamoto, G.C. Thiang, P. Pirro, K.-W. Kim, K. Everschor-Sitte, and E. Saitoh, Topological characterization of classical waves: The topological origin of magnetostatic surface spin waves, Phys. Rev. Lett. **122**, 217201 (2019).

[3] T. Yu, Z. Luo, G.E.W. Bauer, Chirality as generalized spin–orbit interaction in spintronics, Physics Reports **1009**. 1 (2023).

Correlation among magnetic field, spin fluctuation, and electric polarization exhibited by electronic ferroelectric oxide RFe2O4 in nonmagnetic state

Naoshi Ikeda
Grad. Sch. of Env. Life. Nat. Sci. and Tech., Okayama Univ., Okayama, Japan
*E-mail: ikedan@okayama-u.ac.jp

Rare-earth mixed valence iron oxide RFe_2O_4 (R=In, Sc, Y, Dy, …, Lu) was discovered in 70s, and intensive studies were performed in relation to the Verwey type transition irons[1]. Through neutron diffraction and Mössbauer spectroscopy research, the polar charge ordering model was proposed in relation to the spin ordering of iron in this material [2,3,4]. If the electric polarization which arises from the polar electronic order really exist, we could be expected unique and interesting properties which may expand the field of ferroelectricity[5]. With such interests, we performed a Resonant X-ray Scattering (RXS) experiment and found the existence of polar charge ordering in $LuFe_2O_4$, in which the super lattice of Fe^{2+} and Fe^{3+} loses inversion symmetry in iron triangular lattice[6].

However, the clear indication of the macroscopic spontaneous electric polarization had long been not reported. In 2016, it was reported that the RFe_2O_4 has the tendency to form the iron vacancy, and when the stoichiometry of the Fe is completed, the long range coherence of the spin and charge order develops[7]. So the investigation of nonlinear optical (Second Harmonic Generation, SHG) measurement for such a stoichiometric crystal successfully found out the existence of the spontaneous electric polarization below 400K[8].

It is expected that the electric polarization arising from the polar electronic ordering may exhibit unique physical properties such as the ultrafast response of electric dipole, magneto-electric interacted phenomena, and so on. In this talk, we present recent research results of such properties of electronic ferroelectric behavior of RFe_2O_4[9,10]. Specially, recent discovery of the unique coupling between lattice modulation and magnetic field would be discussed.

This coupling between the magnetic field and the lattice is found just the above magnetic transition temperature. We consider that the phenomena has new but complicated mechanism. We are assuming on the mechanism as that the magnetic field suppresses the spin fluctuation in the short-range spin ordering embedded in iron polar charge ordering region, inhibits the development of the electric polarization, which causes the lattice distortion.

[1] N. Kimizuka, *et al.*, *Solid State Commun*. 15, 1199 (1974).
[2] K. Siratori, *et al.*, *Ferrites Proc. ICF 6*, 703 (1992).
[3] M. Tanaka, *et al.*, *J. Phys. Soc. Jpn*. 58, 1433 (1989).
[4] N. Ikeda, *et al.*, *Ferroelectrics* 161, 111 (1994).
[5] Yasusada Yamada, *J. Korean Phys. Soc.*, 32, S1~S4 (1998)
[6] N. Ikeda, *et al.*, *Nature* 436, 1136 (2005).
[7] K. Fujiwara, *et al.*, *Trans. Mat. Res. Soc. Jpn*. 41, 139 (2016).
[8] K. Fujiwara, *et al.*, *Sci. Rep.* 11, 4277 (2021).
[9] H. Yu, *et al.*, *Materials* 16, 1989 (2023).
[10] H. Yu,, *et al.*, *Phys. Rev. Materials* 8, 064402 (2024).

Singular continuous and nonreciprocal phonons in quasicrystal

Masato Matsuura[1*], Zhang Jinjia[2], Yasushi Kamimura[2], Maiko Kofu[3], Keiichi Edagawa[2]

[1]Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS), Tokai, Ibaraki 319-1106, Japan
[2]Institute of Industrial Science,The University of Tokyo, Komaba, Meguro-ku, Tokyo 153-8505, Japan
[3]*J-PARC Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan*

*E-mail: m_matsuura@cross.or.jp

Since quasicrystals lack the translational symmetry of crystals and exhibit quasiperiodic long-range order, they are expected to exhibit exotic physical properties not found in crystals. Although the understanding of the static structure of quasicrystals has been advanced with higher dimensional spaces, the understanding of the dynamic response of quasicrystals is still not satisfactory.

The lattice dynamics of quasicrystals consist of phonons and phasons, which corresponds to excitations in real and complementary space, respectively. The most characteristic feature of the phonons in quasicrystals is a gap feature at the so-called pseudo Brillouin zone boundaries (PBZB), which positions are defined by $q_{\mathrm{PBZB}} = Q_{\mathrm{Bragg}}/2$. Early studies of i-AlPdMn in 90's did not find a clear gap [1]. Later, a clear pseudogap was observed by using inelastic X-ray scattering in both i-ZnMgSc quasicrystal and ZnSc 1/1 approximant[2]. However, these pseudogaps were observed at q= 0.5~0.7 $Å^{-1}$, corresponding to the wave length of 10~12 Å. At such short scales, the aperiodic features may not appear clearly.

In order to seek for lattice dynamics related to aperiodicity, we focused on phonons at low-energies because it reflects dynamics at larger scale. By using the state-of-the-art neutron time-of-flight spectrometers DNA and AMATERAS at J-PARC, we studied the acoustic modes in i-AlPdMn with various energy resolution extending from 0.003 to 1.4meV [3]. We found hierarchical dip structures in the acoustic mode, which are scaled by golden mean τ. This τ-scaling in the dip energies strongly indicate the observed dip feature are related to aperiodicity. Furthermore, asymmetric signals were found in both Q and energy, indicating characteristic nonreciprocal phonon propagation in quasicrystals.

[1] Marc de Boissieu et al., J. Phys: Cond. Mater. 5, 4945 (1993).
[2] Marc de Boissieu et al., Nat. Mater. 6, 977 (2007).
[3] M. Matsuura et al., to be published in Phys. Rev. Lett.

Atomistic modeling of mechanical properties of base-centered cubic multi-component alloys

I. Lobzenko[1*], T. Tsuru[1]

[1]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan
*E-mail: lobzenko.ivan@jaea.go.jp

Refractory multi-component alloys (MCA) have base-centered cubic (BCC) structure and form an important class of materials with high potential for use in severe conditions. It is well known that the static and dynamic properties of dislocations have a crucial effect on the mechanical properties of metals and alloys. The low energy of nucleation and movement of the screw dislocations in ZrNbTaTiHf is the reason for ductility at room temperature [1], so the properties of dislocations define the brittle-to-ductile transition temperature (BDTT). In the present study, to achieve high accuracy in classical molecular dynamics simulations of dislocation motion, we apply the technique of machine learning for interatomic potential development. The influence of datasets on the reliability of machine-learning potentials (MLPs) is discussed. Results of modeling movement of dislocation with MLPs in MoNbTa and ZrNbTa are shown in Fig. 1. The unusual (112) slip plane, which is different from the usual 110 slip plane in single BCC metals, can be seen.

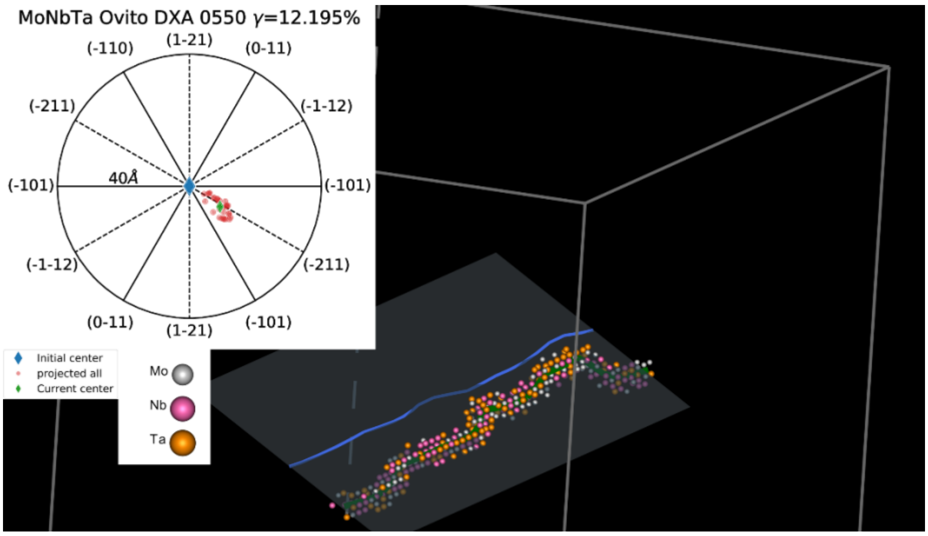

Fig.1: Screw dislocation kink-type glide on a (112) plane in MoNbTa MCA.

[1] T. Tsuru, S. Han, S. Matsuura, Z. Chen, K. Kishida, I. Lobzenko, S. Rao, C. Woodward, E. George, H. Inui "Intrinsic factors responsible for brittle versus ductile nature of refractory high-entropy alloys" // Nature Communications, **15**, 1706 (2024).

Thermodynamic formation mechanism of nitride nano cluster in iron

M. Enoki[1*], H. Ohtani[2]

[1]Shimane Univ., Faculty of materials for energy, Matsue, 690-8504, Japan
[2]Toyota PCRI, Nagakute, 480-1192, Japan

*E-mail: masanori.enoki@mat.shimane-u.ac.jp

Next-generation automobiles require surface hardening materials for high-torque gearboxes with excellent fatigue and wear resistance. Recent studies have confirmed the presence of nanoclusters in steels, formed by substitutional and interstitial solute elements, which significantly enhance surface hardness [1]. To leverage this mechanism, it is crucial to predict the clustering ability of these elements. We employed first-principles calculations of solute atom distributions to predict microstructures based on alloy composition and heat treatment. The thermodynamic basis of cluster formation was analyzed using free energy data from these calculations.

A two-sublattice model in BCC Fe was used, with N and vacancies in octahedral interstitial sites, and Ti in Fe atomic sites. Various ordered structures were evaluated through first-principles calculations, and effective cluster interactions were derived using the cluster expansion method. Monte Carlo (MC) simulations were then used to study the equilibrium distribution of solute atoms at different temperatures, with N concentration controlled by the chemical potential difference ($\Delta\mu$) between N and vacancies. Ti content was varied from 1% to 5% in 1% intervals. Data on solute distribution were collected by changing the temperature from 400 to 1000 K in 50 K steps.

Figure 1 shows results for Fe-1at.%Ti at 500 K. Figure 1(a) depicts the equilibrium N concentration as a function of $\Delta\mu$, with N concentration increasing as $\Delta\mu$ increases. Figures 1(b) and 1(c) show equilibrium atom distributions for $\Delta\mu$ = 200 meV and $\Delta\mu$ = 300 meV, respectively. N atoms are gray, and Ti atoms are light blue. Figure 1(b) replicates the plate-like clusters observed experimentally, while Figure 1(c) shows a uniform Ti distribution. Higher N concentration leads to smaller Ti clusters surrounded by N, inhibiting plate-like cluster formation. In the presentation, similar calculations are used to discuss the short-range ordering in high-entropy alloys (HEAs).

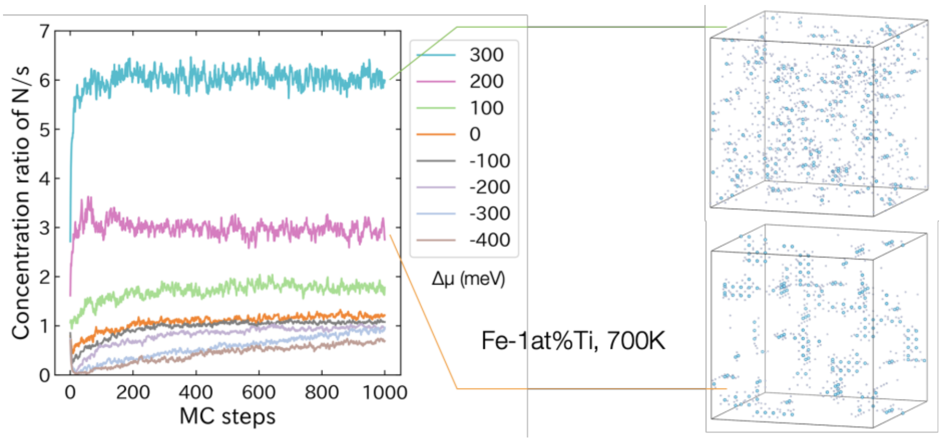

Fig.1: Results of calculations for the Fe-1at.%Ti alloy performed at T = 500 K.

[1] G. Miyamoto, Y. Tomio, H. Aota, K. Oh-ishi, K. Hono, and T. Furuhara, et al., Mater. Sci. Tech., 27(2011)

Search for Significant Short-Range Ordering in Medium-Entropy Alloys

Yoichi Ikeda[1*], Saiki Futami[2], Hong-Fei Zhao[2], and Masaki Fujita[1]

[1]Institute for Materials Research, Tohoku University, Sendai, Japan
[2]Graduate School of Science, Tohoku University, Sendai, Japan
*E-mail: yoichi.ikeda.d2@tohoku.ac.jp

The short-range ordering (SRO) phenomenon is a classical issue in the field of metals and alloys, such as Cu-Ni and Cu-Pd, and is once again in the spotlight, especially in high-entropy alloys. Recently, leading scientific journals have considered SRO to be a key factor in achieving a good balance between strength and toughness or ductility. However, these reports lack significant evidence linking SRO to these properties [1]. Therefore, it is necessary to quantify SRO to reveal the true relationship between SRO and the mechanical and alloy properties. The goal of SRO research is to evaluate the degree of SRO and to develop a methodology for evaluating SRO parameters using experimental techniques. To address this challenge, our recent research [2-4] aims to evaluate the Warran-Cowley SRO parameters using neutron scattering (pair distribution function) data and real-space structure modeling.

Figure 1 (left) shows the reduced pair distribution function data of the quenched Mn-Co-Ni medium-entropy alloy. For a fully random FCC structure, the height of $G(r)$ at the 1st and 2nd neighbor positions should be almost 2:1 because of the difference in coordination numbers at these positions. A similar height of $G(r)$ at these positions may indicate the existence of concentration modulation in an atom-scale region. To evaluate possible types of atom pair segregation, we attempted to determine WC-SRO parameters from our superstructure model, which was constructed using the reverse Monte Carlo method. The evaluated WC-SRO parameters are shown in Fig. 1 (right). At the nearest neighbor (N.N.) positions, the Mn-Ni atom pair is favored, while Mn-Mn and Ni-Ni pairs are favored at the next-nearest neighbor (N.N.N.) sites. The qualitative features of SRO in Mn-Co-Ni seem to be consistent with the theoretical estimations [5]. In this workshop, we will also discuss the results for other medium-entropy alloys, such as the prominent Cr-Co-Ni alloy.

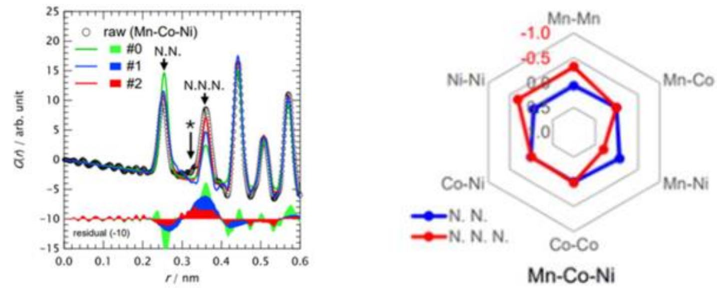

Fig. 1 Evaluated SRO parameters of Mn-Co-Ni (All data were cited from ref. 2).

This research was supported by JSPS KAKENHI Grant Number (JP19H05164 and JP21H00139), and partly by JP24K01143. Experiments were performed under a user program of MLF J-PARC (2020A0276), and ISSP at JRR-3 (6G IRT Program 23402).We gratefully acknowledge support from the Center of Neutron Science for Advanced Materials, Institute for Materials Research, Tohoku University.

[1] R. Zhang et al., Nature **581**, 283 (2020); Note that a part of the report is later challenged by negative findings reported subsequently, as is frequently observed in such papers. [2] S. Futami *et al*., Mater. Trans. **65**, 995 (2024). [3] Y. Ikeda *et al*., Mater. Trans. **64**, 2254 (2023). [4] Y. Umemoto *et al*., Mater. Trans. **64**, 2018 (2023). [5]] M. Mizuno *et al*., Phys. Rev. Mater. **8**, 013601 (2024).

Inelastic X-ray and Neutron Scattering of High-Entropy Alloys

S. Tsutsui[1, 2]

[1]Japan Synchrotron Radiation Research Institute (JASRI), SPring-8, Sayo, Hyogo, Japan
[2] Institute of Quantum Beam Science, Graduate School of Science and Engineering, Ibaraki University, Hitachi, Ibaraki, Japan
*E-mail: satoshi@spring8.or.jp

Much attention has been paid to excellent mechanical properties of a series of high-entropy alloys as promising structural materials for recent decades [1, 2]. The entropy in the name of alloys is derived from configuration entropy. In these alloy systems, one crystarographic site are shared with several atoms. The concept of high-entropy alloy has also been applied to exploring novel fucntional materials such as superconducting compounds, catalysts, and so on.

Phonon dispersion relations are helpful to understand origin of mechanical properties in materials on microscopic viewpoints. However, analyses of dynamical structure factors have not been established in high-entropy alloys theoretically and experimentally. Nowadays, we have two techniques, inelastic X-ray and neutron scattering, to elucidate dynamical structure factors in materials, connected with phonon dispersion relations. Since scattering cross section of phonons differs between X-rays and neutrons, comparison of dynamical structure factors obtained by inelastic X-ray and neutron scattering enables us to understand element-specific roles in the excellent mechanical properties in high-entropy alloys microscopically.

In this talk, correlations between mechanical properties and phonon dispersion relations will be discussed through dynamical structure factors obtained by inelastic X-ray and neutron scattering techniques.

[1] J.-W. Yeh, *et al.*, Adv. Eng. Mat. **5**, 6 (2004).

[2] B Cantor *et al.*, Mat. Sci. Eng. **A375-377**, 213 (2004).

Spin-dependent transport in the ferromagnetic high-entropy alloy thin films incorporating heavy metal

Kazuya Z. Suzuki [1],Koki Takanashi[1,2]
[1] Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan2
[2]Advanced Institute for Materials Research, Tohoku University, Sendai, Japan

High-entropy alloys (HEAs) have attracted considerable attention because of their excellent mechanical, heat-, corrosion-, and irradiation-resistance properties. Most studies have focused on their applications as structural materials. However, ferromagnetic HEAs may also exhibit excellent electromagnetic functions which are not observed in conventional alloys. In this study, we focused on the FeNiCoCuPd-HEAs[1], which exhibit Curie temperatures higher than room temperature and contain Pd as a heavy metal with a large spin-orbit interaction In this presentation, we report the spin-dependent transport properties of FeNiCoCuPd thin films fabricated using a sputtering method. This research was partly supported by the JSPS Grants-in-Aid for Scientific Research 21K18180.

[1] Primoz Kozelj et al.Adv. Eng. Mater. 2019, 21, 1801055

High-resolution visualization of the anomalous Nernst effect using AFM tip-induced local temperature gradients

Hironari Isshiki

Insttute for Solid State Physics, Univ. of Tokyo, Kashiwa, Japan
(Current afferiation: Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan)
*E-mail: h_isshiki@issp.u-tokyo.ac.jp

We have developed a novel method to visualize the anomalous Nernst effect (ANE) using an atomic force microscope (AFM) [1, 2]. In this method, a local temperature gradient is created by contacting an AFM probe with a heated sample wire, as shown in Fig. 1. We detect the voltage resulting from ANE at both ends of the sample wire, enabling magnetic imaging with a spatial resolution of ~80 nm. This method was applied to the antiferromagnetic Weyl semimetal Mn_3Sn. Figure 2 presents the results for Kagome-in-plane textured polycrystalline Mn_3Sn [3]. As seen in Figs. 2(b) and 2(c), the local ANE, corresponding to the distribution of the cluster magnetic octupoles in Mn_3Sn, was observed in both the initial and residual states. Furthermore, this method is applicable to a wide range of other materials and devices. In this presentation, we will report on these results and demonstrate the high versatility of the method.

This work was partially supported by CREST (Grant No. JPMJCR18T3) from JST, JSPS KAKENHI Grant-in-Aid for Scientific Research(C) (Grant Nos. 19H05629), Steel Foundation for Environmental Protection Technology.

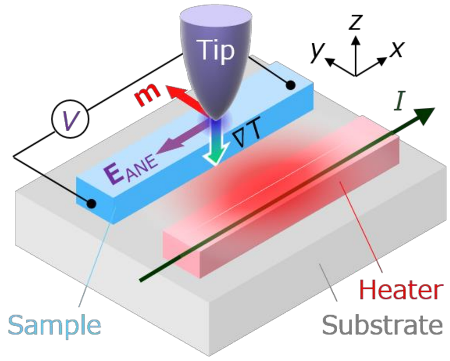

Fig. 1: Schematic diagram of the anomalous Nernst effect mapping.

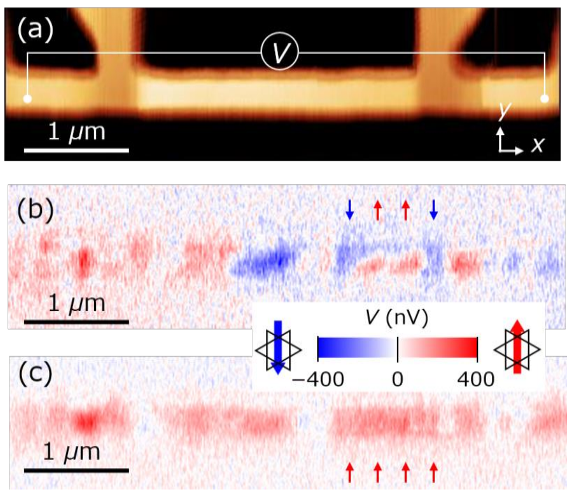

Fig. 2: Results on a Mn_3Sn nanowire. (a) Topography. (b), (c) Results of the anomalous Nernst voltage mapping in the initial and residual states, respectively.

[1] N. Budai et al. Appl. Phys. Lett. 122, 102401 (2023)
[2] H. Isshiki et al. Front. Phys., 11 (2023)
[3] H. Isshiki et al. Phys. Rev. Lett. 132, 216702 (2024)