	Sunday, Feb. 3	
15:00 -	Registration (Hotel Ocean)	
17:00 -	Get Together	

			Monday, Feb. 4	
09:00	-	09:20	Registration (U. of Ryukyus)	
09:20	-	09:30	Opening	
			Plenary Talk	Chair: Ki Bong Lee
09:30	-	10:00	Being and Non-being	Prof. Susumu Ikeda
				(KEK)
10:00	-	10:20	Facility Report	Yasuhiko Fujii
			Promotion of Public Utilization of Large Facilities for Small	(CROSS-Tokai)
			Science	
			Coffee Break (15min)	
		40 ==	Facility Report (cont'd)	Chair: Yasuo Endo
10:35	-	10:55	Present status of J-PARC	Masatoshi Arai
10.55		44.45	Currying Northern Crience and Facility at HANARO	(JAEA/J-PARC)
10:55	-	11:15	Growing Neutron Science and Facility at HANARO	Kye Hong Lee
11:15		11:35	Noutron Possarch Activity in KLIPPI	(KAERI)
11.15	-	11.55	Neutron Research Activity in KURRI	Yuji Kawabata (Kyoto Univ.)
11:35	_	11:55	Current Status of JRR-3 and its Engineering	Hiroshi Suzuki
11.55		11.55	Current Status of Jint-5 and its Engineering	(JAEA)
11:55	-	12:10	Photo Session	(57 127 1)
12:10	-	13:30	Lunch/Business Meeting	
			Instrumentation I	Chair: Je Geun Park
13:30	-	13:55	Powder Diffraction for Materials Research	Takashi Kamiyama
				(KEK)
13:55	-	14:20	The current status and recent results of iMATERIA	Toru Ishigaki
				(Ibaraki Univ.)
14:20	-	14:45	IBARAKI Biological Crystal Diffractometer (iBIX) at J-PARC	Ichiro Tanaka
				(Ibaraki Univ)
			Coffee Break (15min)	
			Hard Matter	Chair: Shinichi Itoh
15:00	-	15:25	Common understanding of magnetoelectricity in various	Jae-Ho Chung
			types of hexaferrites	(Korea Univ.)
15:25	-	15:50	Structural distortion driven by quadrupole ordering of	Kun-Pyo Hong
45.50		46.1-	PrB6	(IBS, CFICES, SNU)
15:50	-	16:15	Spin dynamics of room-temperature multiferroic BiFeO3	Jaehong Jeong
				(Seoul National Univ

# **Banquet (Ryukyu Style Restaurant)**

			Tuesday Feb 5	
			Tuesday, Feb. 5	
			Instrumentation II	Chair: Takashi
00.00		00.05		Kamiyama
09:00	-	09:25	Wide and Small Angle Neutron Scattering for the Study of	Baek-Seok Seong
00.25		00.50	Engineering Materials	(KAERI)
09:25	-	09:50	Neutron Brillouin Scattering on HRC	Shinichi Itoh
09:50		10.05	The first result of the diely shapper time of flight	(KEK)
09.50	-	10:05	The first result of the disk chopper time-of-flight spectrometer DC-ToF at HANARO	Ji-Yong So (KAERI)
			Coffee Break (15min)	(NAENI)
			Soft Matter	Chair: Ichiro Tanaka
10:20	_	10:45	Neutron Studies on the Stimuli-Triggered Structural	Kookheon Char
10.20	_	10.43	Changes in Functional Polymer Platforms	(Seoul National Univ.)
10:45	_	11:10	Periodic distribution of ions confirmed by contrast	Koichiro Sadakane
10.43		11.10	matching small-angle neutron scattering in water, organic	(KEK)
			solvent, and salts	(NEN)
11:10	_	11:35	Neutron Reflectivity Study of Thin Film Polymer	Jaseung Koo
			Multilayers in Supercritical Carbon Dioxide	(KAERI)
11:35		12:00	Small Angle Neutron Scattering Study of Phase Behaviors	Tae-Hwan Kim
11.55	-	12.00	of Amphiphilic Molecules in Aqueous Solution	(KAERI)
12:00	_	13:30	Lunch	(KALNI)
12.00		13.30	Instrumentation III	Chair: Jae-Ho Chung
13:30	_	13:55	Current Status of the Si Crystal Analyzer near	Nobuaki Takahashi
13.30		13.33	Backscattering TOF Spectrometer DNA in a Spallation	(JAEA/J-PARC)
			Neutron Source at J-PARC	(67.127.40.77.11.0)
13:55	-	14:20	Polarized 3He neutron spin filter - development and	Takashi Ino
			application	(KEK)
14:20	-	14:45	Nuclear Data Measurements using the ANNRI in J-	Atsushi Kimura
			PARC/MLF	(JAEA)
			Coffee Break (15min)	
			Nano/Industry	Chair: Han Ki Yoon
15:00	-	15:25	Current status and activity on Engineering Materials	Jun Abe
				(JAEA)
15:25	-	15:50	In situ neutron diffraction scattering study of thermal	In Hwa Cho
			decomposition of LiBH4 mixed with modified MWCNT	(KAERI)
15:50	-	16:15	New iron-based mixed-polyanion cathodes for lithium and	Kisuk Kang
			sodium rechargeable batteries: Combined first principles	(Seoul National Univ.)
16.45		16.40	calculations and experimental study	Vana Nama Charl
16:15	-	16:40	Investigation of Hydrogen Storage Mechanism in nano-	Yong Nam Choi
16.40		17.05	porous materials by in-situ neutron scattering	(KAERI)
16:40	-	17:05	Small Angle Neutron Scattering Study of Nano Sized Microstructure in Ferrous Alloys	Young-Soo Han (KAERI)
			Closing	(NAENI)
			Farewell Dinner	
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#### Oral-OP01

### Being and Non-being

#### S. Ikeda

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The first small Korea-Japan meeting was held at KEK with invitation of two Korean scientists and several Japanese scientists. The purpose was to establish fruitful collaboration in neutron science between both countries. Ever since eleven meetings have been held in Korea- and Japan-sites, and developed many friendly collaboration as well as grown up many young scientists. This attempt was a great success as the first stage. Now a day, other techniques as light sources are developing much quickly. Therefore, it is always expected that neutron methods and technologies should be innovated toward the new science fields, and that advantages of neutron techniques can be claimed more strongly and clearly, comparing with other techniques 'abilities. It also means that the existing or non-existing of neutron science itself should be considered again from the beginnings at all times. For such great innovation, the second stage should beplaned under the strong collaboration of Korea and Japan.

### Promotion of Public Utilization of Large Facilities for Small Science

#### Y. Fujii

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Neutron scattering and synchrotron radiation researches are categorized into "Small Science", which can be conducted by a small number of researchers/students, even by a single person. However, it requires such a "Large Facility" as nuclear reactor or accelerator, which costs a large amount of taxpayers' money not only for construction but also for operation. On the other hand, the nuclear or high-energy physics experiment is conducted by a large number of researchers with their common purpose, for example, to discover an unknown particle based on a large scale facility. This is called "Large Science at Large Facility" in contrast to "Small Science at Large Facility".

The "Small Science at Large Facility" covers a wide variety of research fields ranging from basic/applied research to industrial/medical application; therefore, it plays a central role in promoting science and technology in the nation. For such a purpose it is essentially important to secure a stable and reliable operation of the Large Facility for Small Science. The Japanese Government recently introduced the Legislation for the "Promotion of Public Utilization of Specific Advanced Large Research Facilities", which has been successfully applied to the neutron facility of J-PARC/MLF, the synchrotoron/X-FEL facility at SPring-8/SACLA, and the super-computer facility at K-Computer. This legislation requires that at the "Specific Neutron Beam Facility", an independent thirdparty organization (known as the "Registered Institution") should manage and execute the activities associated with the selection of research proposals for, and the support of user experiments on the public beamlines in preference to the original builder and installer of these facilities (JAEA). Similarly, the role of the Registered Institution will include also activities associated with the selection and implementation of proposals to build contract beamlines put forward by other organizations and with a periodic review of their activities after the construction.

CROSS-Tokai was selected by the Ministry for Education, Culture, Sports, Science and Technology (MEXT) as the "Registered Institution" for this purpose and formally appointed by the Minister on the 22<sup>nd</sup> of March, 2011. Accordingly, on the 1<sup>st</sup> of April, 2011, CROSS-Tokai assumed this role and began operations at its offices within the JAEA precinct. Thus this legislation secures the operation of the Specific Advanced Large Research Facility after its construction with respect to its finance and man power.

# Status Report of J-PARC MLF (The Materials & Life Science Experimental Facility)

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J-PARC MLF was designed to be a 1 MW spallation neutron source. The averaged neutron flux is about 1/4 of ILL research reactor. However, the pulse peak flux can exceed 100 times that of ILL. This factor gives new paradigm for neutron scattering not only in basic science but also in application such as industrial use of neutrons. Present power of the proton accelerator is 300 kW with a very stable operation, 94% world-level stability, after recovering from the devastating disaster happened in March two years ago. Therefore users have enjoyed their experiments very much. It is planned to increase the power to be 400 kW after the summer shutdown, when we will upgrade accelerator. 20 instruments have been already funded, 16 are available for user program and four instruments are under either commissioning or construction. Operational time for user program in 2012 is about 180 days, and we have received more than 550 experimental proposals from users. World-class scientific outputs have been already created in various scientific fields, ranging from Li-battery science to bio-molecular science. Since J-PARC is internationally open for users, we have got experimental proposals from abroad more than 10% of the whole proposals. More than 30% of proposals have come from industries, such as Toyota, Nissan, Honda, Panasonic and other big industries. This fact has revealed a new horizon come in the neutron scattering science in the 21 century. We are expecting those statistics will increase more than three times at 1MW in three to four years time.

In my talk, I will describe not only on current status of J-PARC MLF neutron source but performance of instruments and scientific topics.

## **Growing Neutron Science and Facility at HANARO**

K. H. Lee Korea Atomic Energy Research Institute, Daejeon, Korea Email: khlee@kaeri.re.kr

Three more cold neutron instruments, REF-V, DC-ToF, and USANS, have been open to users in 2012 following two SANS' open in 2010. In 2013, 2 thermal neutron instruments, Bio-D and Bio-C and cold TAS, cold neutron PGAA and Neutron Depth Profiling will be open to users. 17 neutron instruments will be running in the reactor hall and guide hall at the end of 2013. The number of users in 2011 was 500 and it will be increasing as more neutron instruments are open and the reactor operation becomes stable.

It is very encouraging that Institute for Basic Science included neutron science as one of its research centers. Currently, there are 280 members in Korea Neutron Beam Users Association, but the neutron community will obviously grow as more research fund is put into this research area through IBS.

What is not in a sound situation is a user program, through which more advancement and improvement of the instruments and sample environment should be performed and more instrument scientists and engineering support staff should be secured.

# **Neutron Research Activity in KURRI**

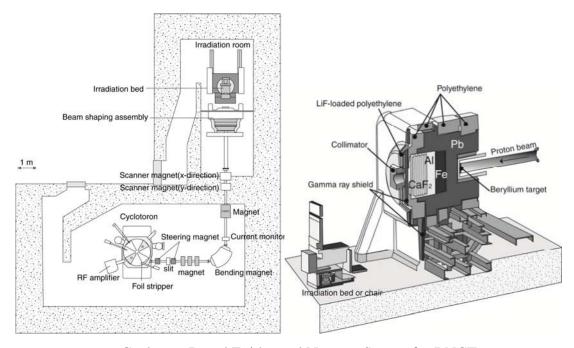
#### J.Kawabata

Research Reactor Institute, Kyoto Univ., Kumatori, Osaka, Japan Email: kawabata@rri.kyoto-u.ac.jp

KUR has been operated without any problem though we had a very big earthquake and Fukushima accident in 2011. It is the only MW class research reactor operated in Japan now. The number of proposals for KUR experiment are recovered after the 4 years(2006 spring - 2010 Spring) interruption for the fuel conversion.

The accelerator-driven system (ADS) using the complex of a Fixed Field Alternating Gradient (FFAG) proton accelerator and Kyoto Univ. Critical Assembly (KUCA) is also operated constantly for nuclear physics experiments. A BNCT facility with a cyclotron base neutron source was installed in 2008 and the clinical trials for the

human therapy started in October 2012 after a long commissioning and animal trials.



Cyclotron Based Epithermal Neutron Source for BNCT

## **Current Status of JRR-3 and its Engineering Diffractometers**

<u>H. Suzuki,</u> S. Wakimoto, H. Matsue, M. Shibayama<sup>1)</sup> and K. Kakurai

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Instruments in the JRR-3 have been continuously upgraded, and produced many interesting results in research fields of materials and life science under the National Universities' Users Program and the JAEA User Program. Recently, many users from industries come to use neutrons for their researches and developments. Especially the neutron engineering diffractometers, RESA-1 and RESA-2, are often utilized for measuring residual stresses as well as for evaluating materials strengths in their products. However, the JRR-3 has been out of service for a long time due to the earthquake occurred on March 11<sup>th</sup>, 2011. First of all, we would like to acknowledge neutron facilities abroad including the HANARO and neutron colleagues for many offers of acceptance of JRR-3 proposals after the earthquake.

The damage of instruments in the JRR-3 due to the earthquake was not so serious, so fortunately they have already been recovered from the disaster. However, lost alignment in neutron guide tubes estimates about 85% neutron flux of before the disaster after the realignment. Meanwhile, we have undertaken not only recovery but also improvement, e.g., replacing the cold neutron guides, C1 and C3 lines, with the supermirror guide tube for increasing their neutron flux. The JRR-3 has not restarted yet, but all instruments are ready to accept the neutrons. On the other hand, the JRR-3 Users Office was started in Apr., 2010 to provide user supports for 18 instruments owned by the JAEA. They have recently worked to improve the user-interface like establishments of the JRR-3 publication database and the new proposal application system, RING [1], by organizing some working groups. Furthermore, they have dedicated their efforts to internationalization for accepting international users in near future, e.g., building the JRR-3 facility homepage [2] and the Users Office homepage [3] in English.

In this presentation, we will introduce current status of the JRR-3 after the earthquake including present user support system as well as some research topics especially in neutron engineering diffraction.

- [1] RING: https://jrr3ring.jaea.go.jp/index.php (in Japanese only)
- [2] JRR-3 facility homepage: <a href="http://jrr3.jaea.go.jp/jrr3e/index.htm">http://jrr3.jaea.go.jp/jrr3e/index.htm</a>
- [3] JRR-3 Users Office homepage: <a href="http://jrr3uo.jaea.go.jp/jrr3uoe/index.htm">http://jrr3uo.jaea.go.jp/jrr3uoe/index.htm</a>

#### **Neutron Powder Diffraction for Materials Research**

Takashi KAMIYAMA, Masao YONEMURA, Shuki TORII, Ryoko TOMIYASU, Yoshihisa ISHIKAWA

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MLF (Materials and Life Science Facility) of J-PARC has six neutron powder diffractometers (NPD's) with different resolution, intensities, and apparatuses for pursuing different research subjects. All NPD's have the potential to explore the science regions not possible with conventional NPD. SuperHRPD is the highest resolution NPD and is able to detect tiny structural change during phase transition, and to determine crystal structures of complex materials of interest. Various *in situ* studies and/or real time studies of functional materials is more and more important in materials research, and NOVA (a high intensity total diffractometer) and SPICA (a special environment diffractometer) will contribute to the studies of hydrogen absorptions/desorptions, charge/discharge processes, chemical reactions, syntheses, *etc.* We will show some examples.

#### The current status and recent results of iMATERIA

Toru Ishigaki,
Akinori Hoshikawa, Kenji Iwase, Dyah. S. Adipranoto
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iMATERIA (IBARAKI Materials Design Diffractometer) is a high throughput-versatile neutron diffractometer in J-PARC, build by Ibaraki prefecture, the local government of the area where J-PARC sites. It covers the d in range 0.18 < d (Å) < 5 with d/d = 0.16 % at high resolution bank, and 5 < d (Å) < 40 with the resolution changing gradually at two detector banks of 90 degree, and low angle. So, this diffractometer covers very wide drange (0.18 < d (Å) < 40). If the small angle detector bank will be available, which is currently under commissioning, iMATERIA will cover wider d-range (0.18 < d (Å) < 800). It takes several minutes to obtain a "Rietveld-quality" data for the X-ray laboratory sized sample measured at 1MW. Currently, the beam power is limited for tuning the accelerator ( 300kW), so that the measuring time is about 15 to 30 min for standard oxide samples. The automatic sample changer system [2] is most important sample environment for high throughput experiments. The automatic sample changer system consisted of large number of sample storage and two lines of elevating system, pre-vacuum chambers and sample rotating ta-bles. So, this we c an handle more than 600 samples continuously at room temperature without breaking a vacuum of sample chamber. Another standalone sample changer and the cryofurnace with sample changer are also prepared. The analysis software is also very important for powder diffraction data; so that we prepare several powder-diffraction software, include Rietveld analysis software (Z-Rietveld [3,4]) and Maxmum Entropy Method software (Z-MEM). The current status of iMATERIA and the recent data, include the challenge for measurement of small amount of sample and organic samples will be reported.

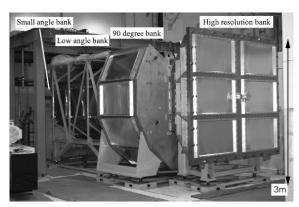


Fig.1 IBARAKI Materials Design Diffractometer, iMATERIA.

- [1] T. Ishigaki et. al., Nucl. Instr. Meth. Phys. Res. A, 600, 189-191 (2009).
- [2] A. Hoshikawa et. al., J. Phys.: Conf. Ser. 251 012083 (2010)
- [3] R. Oishi, et. al., Nuclear Instruments and Methods A 600, 94-96 (2009).
- [4] R. Oishi-Tomiyasu, , et. al., J. Appl. Cryst. 45, 299-308 (2012).

## IBARAKI Biological Crystal Diffractometer (iBIX) at J-PARC

<u>I. Tanaka</u> <sup>AB</sup>, K. Kusaka <sup>B</sup>, T. Yamada <sup>B</sup>, T. Hosoya <sup>AB</sup>, K. Tomoyori <sup>B</sup>, T. Ohhara <sup>C</sup>, K. Kurihara <sup>D</sup>, M. Katagiri <sup>B</sup>, N. Niimura <sup>B</sup>

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Hydrogen, protonation and hydration play important roles in various life processes at the atomic level. In order to study them, a new diffractometer for neutron protein crystallography, IBARAKI Biological Crystal Diffractometer (iBIX), has been constructed at BL03 in the 1st experimental hall of MLF in J-PARC and operational since December 2008[1].

Because of little damage due to the 3.11 big earthquake in 2011, iBIX could start without large troubles. Just before the earthquake, iBIX has succeeded in collecting two data sets; an Alzheimer's disease-related protein and an organic compound with Pb and Br, and their structure analysis results were published in the last year[2, 3].

In the last summer, 16 new detectors were installed and the old 14 detectors were updated to the new system completely so that the iBIX measurement efficiency becomes 3 to 5 times larger than the previous one.

Since autumn of 2012, the J-PARC accelerator power has become 300kW from 200kW. In December 2012, the commissioning and the adjustment of all detectors have almost finished, so iBIX is now expected as one of the highest performance of a single crystal neutron diffractometer in the world.

As recent results, several organic compounds' analyses have finished and test measurements of several proteins have also finished and taking the full data set of them has been on schedule.

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- [1] I. Tanaka, et al., Acta Cryst. D 66, 1194 (2010).
- [2] T. Yokoyama, et al., J. Struct. Biol., 177 (2012) 283.
- [3] T. Kawasaki, et al., J. Phys. Soc. Jpn. 81 (2012) 094602.

ACKNOWLEDGEMENT: The authors thank the Department of planning of Ibaraki Prefectural Government for its sponsorship.

# Wide and Small Angle Neutron Scattering for the Study of Engineering Materials

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Small angle neutron scattering (SANS) and neutron powder diffraction techniques are very powerful tools in determining the size distribution of precipitates and the volume fraction of multi-phases in high strength steels used for automobile bodies. Neutrons make it possible to measure non-destructively in bulk sample with various sample environments such as furnaces, loading devices, cryostats, pressure cells and magnetic fields. In some cases, X-ray, TEM and APT are complementarily used to get the local information in the sample. In this presentation, the quantitative analysis methods of nano-sized precipitates in low carbon steel, the solute carbon content in austenite of TRIP steels, and the partitioning of the martensite phase induced by thermal and mechanical process by neutron scattering techniques performed at HANARO will be introduced.

## **Neutron Brillouin Scattering on HRC**

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Inelastic neutron scattering is a powerful tool for observing coherent excitations in condensed matters. For a single crystalline sample, the dynamical structure factor of the coherent excitations such as magnons and phonons are easily observed by choosing the scattering condition. Contrary to this, measurements of magnetic excitations by using a polycrystalline sample are rather difficult, even though a single crystalline sample is not always synthesized in an early stage of a study in some cases. Scattering intensities of ferromagnetic spin waves from a poly- crystalline sample rapidly decrease as the scattering vector increases from (000) due to the powder average of the dynamical structure factor. It is difficult to access the energy momentum space near (000) and to perform so-called neutron Brillouin scattering (NBS) experiments due to the kinematic constrain of the neutron. To access the energy momentum space close to (000) by an inelastic neutron scattering experiment, neutrons with an energy of sub-eV or higher (incident neutron energy, Ei ) should be incident up on the sample and scattered neutrons should be detected at scattering angles of  $1^{\circ}$  or less with high energy resolution of  $\Delta E$  /Ei being a couple of percent or less.

We here demonstrate NBS experiments on the High Resolution Chopper Spectrometer (HRC) installed at the Material and Life Science Facility (MLF) in Japan Proton Accelerator Research Complex (J-PARC) [1]. The feasibility of NBS on the HRC was demonstrated by observing ferromagnetic spin waves in La0.8 Sr0.2 MnO3 and SrRuO3 polycrystals. Gapless spin-wave excitations were observed in La0.8 Sr0.2 MnO3, which were in good agreement with previous results using single crystals [2,3]. The novel result is a well-defined quadratic Q dependence in the spin-wave dispersion curve with a large energy gap in SrRuO3. We tried to perform preliminary NBS experiments on a polycristalline sample of a permanent magnet Nd2Fe14B. The spin wave intensities were observed at (Q,E) consistent with previous results using single crystals [4]. Also, we performed NBS experiments on liquid D2O. The observed spectra were in good agreement with previous results [5].

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Acknowlegement: This neutron scattering experiment was approved by the Neutron Scattering Program Advisory Committee of the Institute of Materials Structure Science, High Energy Accelerator Research Organization (Proposal Nos. 2011S01 and 2012S01). We are grateful to Y. Kaneko, Y. Tokura, M. Fujita, and K. Yoshida for sample preparations, and to K. Ono and J. G. Park for fruitful discussions. This work was partially supported by Grant-in-Aids for Scientific Research from the Japanese Ministry of Education, Culture, Sports, Science and Technology.

# The First Result of The Disk Chopper Time-of-Flight Neutron Spectrometer DC-ToF at HANARO

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The Disk Chopper Time-of-Flight Spectrometer (DC-ToF) is an inelastic neutron time-of-flight spectrometer using multi-disk choppers and long position sensitive detectors (PSDs) at the HANARO research reactor. The DC-ToF has been developed since 2003 and the first neutrons were observed in Mar. 2012. Since then, the commissioning of the DC-ToF has been taken. This presentation is intended to describe the instrumental specification and performance of the spectrometer. In addition, the first measurement results of standard samples and other samples will be reported.

# Current Status of the Si Crystal Analyzer near Backscattering TOF Spectrometer *DNA* in a Spallation Neutron Source at J- PARC

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A Si crystal analyzer near backscattering spectrometer DNA [1] which covers the area of the micro-eV energy range in the Q-E space, where it is expected to explore sciences on atomic, molecular and spin dynamics in the nanosecond time range has been installed at BL02 of the Materials and Life Science Experimental Facility (MLF) of the Japan Proton Accelerator Research Complex (J-PARC) until at the end of February 2012. Then, various on-beam commissioning has been done for about a year with handling continuing user program. In this report, we will introduce specifications, current status of the instrument.

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# Polarized <sup>3</sup>He neutron spin filter in J-PARC development and application

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The spin-dependent neutron absorption cross section of <sup>3</sup>He nuclei is large enough to realize neutron spin filters (NSFs) from cold to epithermal neutrons with spin-polarized <sup>3</sup>He gas. Such polarized <sup>3</sup>He NSFs are now promising tools for polarized neutron scattering measurements thanks to various technological advances which have improved the <sup>3</sup>He polarization as well as the polarized <sup>3</sup>He gas volume.

The nuclear polarization of <sup>3</sup>He can be achieved by the optical pumping method. The spin-exchange optical pumping (SEOP), in which alkali metal atoms are first polarized through the optical pumping, then their atomic polarization are transferred to <sup>3</sup>He nuclei, and the metastability-exchange optical pumping (MEOP), in which the polarization of metastable helium atoms is achieved and then exchanged with that of the <sup>3</sup>He nuclei, are two popular methods. Each has advantages and disadvantages, but the achieved <sup>3</sup>He nuclear polarizations are essentially the same.

Recent technological developments of <sup>3</sup>He neutron spin filters and application in J-PARC will be presented.

## Nuclear Data Measurements using the ANNRI in J-PARC/MLF

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Accurate neutron capture cross section data for minor actinides (MAs) and long-lived fission products (LLFPs) are required to estimate the production and transmutation rates for developing innovative nuclear systems. However, accurate measurements of these cross sections are very difficult due to high radioactivity of these samples. To satisfy the requirement, Accurate Neutron-Nucleus Reaction measurement Instrument (ANNRI) has been developed in the MLF of the J-PARC. A series of neutron capture cross-section measurements have been started with the ANNRI.

There are two spectrometers in the ANNRI. One is a large germanium detectors array at the flight length of 21.5 m and the other one is a NaI spectrometer at the flight length of 28 m. Using the spectrometers with a neutron time-of-flight method, both energy of neutrons and prompt- $\gamma$  rays are measured at the same time. The energy-integrated neutron intensities at the flight length of 21.5 m are  $1.2\times10^7 \text{n/s/cm}^2$  in the neutron energy range of 1.5-25 meV, and  $1.8\times10^6 \text{n/s/cm}^2$  in 0.9-1.1 keV at a beam power of 300 kW. In the epithermal energy region, the energy-integrated neutron intensity is more than 10 times as high as the values of the other instruments. Moreover, under the future 1-MW operation, these intensities are expected to increase to  $4.3\times10^7$ , and  $6.3\times10^6 \text{ n/s/cm}^2$ , respectively.

Currently, analyses of <sup>244</sup>Cm, <sup>246</sup>Cm and <sup>237</sup>Np have been finished, and analyses of <sup>241</sup>Am, 129I, <sup>107</sup>Pd, <sup>99</sup>Tc and <sup>93</sup>Zr are in progress. These results will make significant contributions in the field of developing innovative nuclear systems. Furthermore, using strong pulsed neutrons, the ANNRI has been used not only for nuclear data but also nuclear astrophysics and microanalysis.

ACKNOWLEDGEMENT: This work is partly supported by JSPS KAKENHI (22226016 and 22760675)

#### Oral-OH01

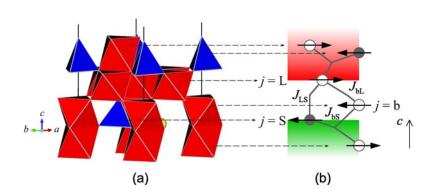
# Common understanding of magnetoelectricity in various types of hexaferrites

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In magnetoelectric multiferroics, electric polarizations can establish without ionic displacements via spin-orbit coupling that involves spin moments with noncollinear spatial arrangements. Practical applications of this novel phenomenon seems imminent thanks to the recent realization of room-temperature magnetoelectricity in hexagonal ferrites[1,2]. So far, field-induced electric polarization has been observed in several polymorphs of hexaferrites. The associated magnetic orderings under external field bear significant similarities in spite of apparent differences in crystal structures.

In this work, we will present recent neutron diffraction works on Y-, Z-, M-, and U-type hexaferrites, and compare the results with field-induced electric polarizations. We will review and compare their crystal structures, and propose the model that can explain the common behavior among different types of hexaferrites. The key idea is the coexistence of easy-plane and easy axis anisotropy fields, which depend on local coordination of  $Fe^{3+}$  (3 $d^5$ ) ions. This model, which involves competing exchange interactions and magnetic anisotropy fields across the interface, may provide further insights into the development of high-performance multiferroics.



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#### Oral-OH02

### Structural distortion driven by quadrupole ordering of PrB6

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Rare-hexaboride has been extensively studied for its unique phase transitions, namely quadrupolar ordering. PrB<sub>6</sub> is one such example with two successive phase transitions[1,2,3,4]. In this talk, we have investigated the structure of PrB<sub>6</sub> throughout the phase transitions using a high resolution powder diffractometer of ISIS.

We have examined carefully the structural changes around the two successive magnetic phase transitions: for example one at 7 K from paramagnetic to incommensurate phases and another one at 4.2 K from incommensurate to commensurate phases. According to our studies, a monoclinic structure,  $P \ 2/m$ , appears with the slight distortion of the cell parameters and boron positions below 4.2 K. Interestingly enough, fluctuations of three boron types were observed along the crystallographic axes.

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#### Oral-OH03

# Spin dynamics of room-temperature multiferroic BiFeO<sub>3</sub>

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Multiferroic compounds are one of promising materials for new spintronic device application such as magnetic/electric memories with the coupling between magnetism and ferroelectricity. Among several multiferroic compounds, BiFeO3 is probably the only exception that has both magnetic and ferroelectric transition above room temperature. It also has the cycloidal spin structure with an extremely long period.

In order to understand the microscopic magnetic interactions in BiFeO3, we have carried out inelastic neutron scattering experiments on several co-aligned single crystals, using three spectrometers: AMATERAS of J-PARC, MERLIN of ISIS and 4F2 of LLB. We employed a so-called sample rotation method for the MERLIN measurements and could measure the magnon dispersion over the full Brillouin zone [1]. We have also examined the detailed structures of the unusual low-energy excitations using the TAS, 4F2.

For the analysis, we have calculated the magnon dispersion and conducted Monte-Carlo simulation using a Hamiltonian with two Heisenberg exchange interaction between the nearest and the next nearest neighbors and a Dzyaloshinskii-Moriya interaction associated with its cycloidal magnetic structure. We could determine the interaction parameters that are consistent with both experimental results and the Monte-Carlo simulations.

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# Neutron Studies on the Stimuli-Triggered Structural Changes in Functional Polymer Platforms

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Our current interests with the CRI Center have been focused on the development of functional polymer platforms whose nanoscale structural changes significantly influence the performance of energy harvesting or biomedical devices. As a result, the control and detailed analysis on the shape and size of functional structures within the thin film platforms are ultimately important for the utilization of such platforms. We have performed both small angle neuron scattering (SANS) and neutron reflectivity (NR), which have spatial resolutions ranging from a few to thousands of nanometers to characterize such polymeric nanostructures and assembling processes triggered by external stimuli. to obtain desired nanostructures in functional polymer platforms, we have systematically induced the structural changes and the assembly of polymeric films based on various stimuli such as external pH, temperature, and specific chemicals. In this presentation, several examples will be given to demonstrate the power of such neutronbased characterizations: SANS analysis on the polymer-assembled structures of organic solar cells and NR measurements on the stimuli-triggered changes in the internal structures of weak polyelectrolyte-based multilayer thin films. These fundamental characterizations, including both SANS and NR, would give us new insights on the design of functional polymer platforms for a host of applications such as energy and biomedical devices.

# Periodic distribution of ions confirmed by contrast matching small- angle neutron scattering in water, organic solvent, and salts

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Mesoscopic structures, such as lamellar, in a mixture of water, 3-methylpyridine, and antagonistic salt, NaBPh4, are discovered in our recent studies [1]. According to theoretical investigations by Onuki [2], hydrophilic and hydrophobic ions tend to adsorb near the interface between water and organic solvent. These ions reduce the interfacial tension between the solvents, and mesoscopic structures are induced [2]. In order to understand the previous experimental results, it is assumed that pairs of hydrophilic (Na<sup>+</sup>) and hydrophobic ions (BPh4<sup>-</sup>) play roles of surface-active agent in a mixture of water and 3-methylpyridine. The details of ion distribution, however, have not been clarified experimentally yet in such mixtures.

In this study, distribution of ions is investigated in a mixture of water (D<sub>2</sub>O + H<sub>2</sub>O), deuterated 2,6-lutidine (2,6-lutidine-d<sub>9</sub>), and NaBPh<sub>4</sub>, instead of a mixture of water and 3-methylpyridine, with employing contrast variation SANS. This mixture also

shows a lamellar structure, which is evident by the SANS measurement as shown in Fig. 1. The first sharp peak originated from the lamellar structure is observed at  $Q = 5.5 \times 10-2 \text{ Å}^{-1}$  even at the matching point. This result indicates that Na<sup>+</sup> and BPh<sub>4</sub><sup>-</sup> ions distribute periodically in a mixture of water and 2,6-lutidine, whose mean repeat distance is approximately 100 Å. In the presentation, we will also exhibit the result of partial scattering function derived from the singular-value decomposition.

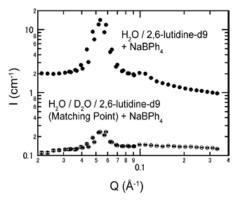


Figure 1: SANS profiles for the mixture of water, 2,6- lutidined9, and NaBPh4.

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# Neutron Reflectivity Study of Thin Film Polymer Multilayers in Supercritical Carbon Dioxide

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We investigated the effect of supercritical carbon dioxide (scCO<sub>2</sub>) on the swelling behavior and diffusion dynamics of polymer thin film. scCO<sub>2</sub>, namely regime at temperatures and pressures above the critical point values, exhibited large density fluctuations resulting in enhancement of the solubility of the polymers, thereby obtaining the significant attention for "a green solvent" in polymer processing and polymer synthesis. In this study, we used the neutron reflectivity which is an ideal tool for *in situ* measurement of polymer multilayer structure in thick-well vessel flushed with CO<sub>2</sub> gases or liquids due to the large penetration depth inherent with neutrons. The results showed that anomalous dilation of polystyrene (PS) was obtained at the ridge (T = 36 °C and P = 8.2 MPa). This excess CO<sub>2</sub> sorption also improved miscibility of thin polymer bilayer, top PS and bottom deuterated polymethyl methacrylate (d-PMMA) layers. In addition, introducing CO<sub>2</sub> enhanced the mobility of polymer chains even near the silicon substrates and the confinement effect due to interaction between polymer chains and substrates was alleviated in scCO<sub>2</sub>.

# Small Angle Neutron Scattering Study of Phase Behaviors of Amphiphilic Molecules in Aqueous Solution

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Amphiphilic molecules such as surfactant and block copolymer self-assemble into various micellar structures in aqueous solution and reveal excellent phase behaviors under various external conditions such as pH, temperature, or additives. Therefore, these amphiphilic molecules have been of great interests in a broad spectrum of potential applications such as nano-building blocks or drug delivery in nano- or bio-science. However, the self-assembled structure of amphiphilic molecules under the various external conditions has not been fully exploited yet. Here a phase behavior of amphiphilic molecules including surfactants and block copolymers at varying additives and temperature has been investigated. To study the self-assembled structure of amphiphilic molecules, small angle neutron scattering (SANS) experiments were conducted at HANARO 40m SANS instrument. The SANS intensity revealed that surfactants and triblock copolymers formed various micellar structures such as sphere, cylinders or vesicles depending on the additive and temperature [1].

[1] T.-H. Kim, Y.-S. Han, B.-S. Seong, and K. P. Hong, Soft Matter, 7, 10070 (2011).

# Investigation of Hydrogen Storage Mechanism in nano-porous materials by in-situ neutron scattering

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The goal of hydrogen storage performance (capacity) by the US DOE has alleviated recently because of the retardation in development of epochal materials. On this account, the hydrogen storage field became a bottleneck of the forthcoming 'hydrogen economy'. One of the main reasons for this situation maybe an unawareness of the storage mechanisms at the moments of hydrogen sorption and desorption. Various efforts have been paid by materials scientists on searching for better materials by trial & errors (synthesis & evaluation) and chemical inspirations, but it was not successful until now.

Nano-porous materials, which store hydrogen molecules via the physi-sorption mechanism, have attracted much attention because of its excellent reversibility (sorption→desorption). In-situ neutron scattering setup has established at HANARO neutron beam instruments (HRPD and DC-TOF). Precise measurement of the temperature (2~320K) and the pressure (0~100 bars) with neutron scattering data enables us to discuss about the behavior of hydrogen at the very moment. Experimental details and results obtained by HRPD and DC-TOF spectrometer on various nano-porous materials, zeolites and MOFs (metal-organic frameworks), will be presented with simple analyses.

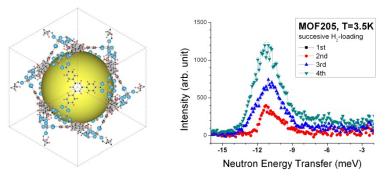


Figure 1. The unit cell structure of MOF205 (left) and rotational transition spectra of  $H_2$  adsorbed on MOF205 at 3.5K (right).

# In situ neutron diffraction scattering study of thermal decomposition of LiBH<sub>4</sub> mixed with modified MWCNT

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LiBH<sub>4</sub> is a promising candidate for the hydrogen storage material due to its extremely high theoretical hydrogen capacity (18 wt.%, 121 Kg m<sup>-3</sup>). However, its practical application has not been easy because of the high reaction enthalpy (~75 kJ mol<sup>-1</sup> H<sub>2</sub>) and the slow hydrogen dissociation kinetics. To addition of catalyst such as MWCNT (multiwall carbon nanotube) is the one way to overcome these problems since the additives can destabilize LiBH<sub>4</sub>, which may reduce reaction enthalpy and increase the surface area of LiBH<sub>4</sub> confining it to nano-sized structures of MWCNT. And it is very important to observe dissociation processes during thermal decomposition of LiBH<sub>4</sub>. In addition, neutron diffraction is powerful tool since neutron can see the signal from hydrogen directly unlike other particles (photon, electron etc.). Our group studied composite system of LiBH<sub>4</sub> mixed with ball-milled MWCNT using in situ neutron diffraction and the effect of the MWCNT is discussed.

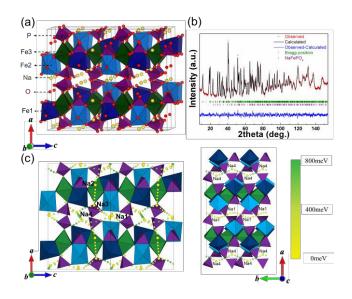
# New iron-based mixed-polyanion cathodes for lithium and sodium rechargeable batteries: Combined first principles calculations and experimental study

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New iron-based mixed-polyanion compounds LixNa4-xFe3(PO4)2(P2O7) (x = 0-3) were synthesized, and their crystal structures were determined. The new compounds contained three-dimensional sodi-um/lithium paths supported by P2O7 pillars in the crystal. First principles calculations identified the complex three-dimensional paths with their activation barriers and revealed them as fast ionic conductors. The reversible electrode operation was found in both Li and Na cells with capacities of one-electron reaction per Fe atom, 140 mAh g-1 and 129 mAh g-1, respectively. The redox potential of each phase was ~3.4 V (vs. Li) for the Li-ion cell and ~3.2 V (vs. Na) for the Na-ion cell. The properties of high power, small volume change, and high thermal stability were also recognized, presenting this new compound as a potential competitor to other iron-based electrodes such as Li2FeP2O7, Li2FePO4F, and LiFePO4.



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# Current status and activity of Engineering Materials Diffractometer TAKUMI at J-PARC

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The Engineering Materials Diffractometer "TAKUMI" which is dedicated to investigate the stress-strain state and the crystallographic structure in engineering materials and/or components was constructed at BL19 in J-PARC/MLF. TAKUMI extracted first beam in October 2008 and the user program started very early in January 2009. Although the Tohoku earthquake occurred in March 2011 and TAKUMI was severely damaged, after the restoration work, TAKUMI has been restored and restarted commissioning in March 2012. In the following month the user program was restarted again.

The best resolution ( $\Delta d/d$ ) and d-range of TAKUMI is 0.17 % and 0.5-2.7 Å (single frame mode), respectively. Radial collimator (gauge width: 1mm, 2mm, 5mm) can be attached to determine the sample gauge volume, which allows strain-mapping measurements of engineering materials. TAKUMI has also several sample environmental devices that realize to perform in-situ neutron diffraction experiments under various conditions. Deformation test up to 50 kN at low temperatures (down to 6K) or high temperatures (up to 1273 K) can be performed. In addition, a texture measurement procedure using a cradle has been also developed to ready for user's experiments.

TAKUMI also has started his upgrading works. A fatigue machine and a stroboscopic measurement method for the fatigue measurements are in under development. A controlling software linking various devices is also under development. Furthermore, a simultaneous measurement system of neutron diffraction patterns and AE (acoustic emission) signals is also developed; AE is elastic wave generated from materials under deformation. This system allows us to measure the strain, acquiring information of the timing, position and propagation of the crack or dislocation generated in the engineering material under stress.

In the presentation, current status of TAKUMI, current sample environments, and several examples performed at TAKUMI, will be introduced.

# Small Angle Neutron Scattering Study of Nano Sized Microstructure in Ferrous Alloys

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The nano sized microstructures in Fe-Cr ODS(Oxide Dispersion Strengthened) alloys and the Fe-Cu alloy were studied by SANS(Small Angle Neutron Scattering). The Fe-Cr ODS steels were manufactured by HIP(Hot Isostatic Pressing) with different chemical compositions and fabrication conditions. The SANS experiments were performed by the 40m SANS instrument at HANARO. Due to the ferromagnetic nature of the ferrous alloys, the horizontal magnetic field of 1 Tesla were applied during the SANS experiment. The nano sized microstructure such as yttrium oxides and Cr-oxides were quantitatively analyzed by SANS in Fe-Cr ODS alloys. The effects of chemical compositions and fabrication conditions on microstructure were discussed according to the quantitative analysis results by SANS. The nano sized Cu clusters were also analyzed by SANS in the Fe-Cu alloy. The effect of heat treatment on microstructure were discussed according to the SANS analysis results in the Fe-Cu alloy. The ratio between magnetic and nuclear scattering components was calculated and the characteristics of the non-magnetic nano sized microstructures in experimental ferrous alloys were discussed from the calculated ratio.

## Universal Event Recording DAQ System in J-PARC/MLF

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We have already implemented the neutron event recording DAQ (data acquisition) system in the neutron experiment instruments at J-PARC/MLF. The neutron signals detected by <sup>3</sup>He-PSDs, scintillators and so on are converted to the digital data by the DAQ electronics and stored into the hard disks of the DAQ computers as the event with TOF (Time Of Flight) and positions. Simultaneously, each neutron production event in the spallation source is recorded with the absolute time. Combining the neutron detection events and the neutron production events, we can recognize when and where each neutron is detected.

In this year, we have introduced the universal signal event recording board which we call "TrigNET" into our DAQ system. The TrigNET has various signal input ports which are 8ch DIOs, 2ch fast ADCs (100MSPS), slow 4ch ADCs (10~1kHz) and the SiTCP interface. The TrigNET can output the event data which consist of the elapsed time from the trigger which indicate a neutron production, the event source and the signal values. We have incorporated the TrigNET with the several instruments and measured the neutron optics device signal, which are the rotating pulse of the choppers, the phase of the neutron polarizer and so on, and the external fields of the sample environment devices which are temperature, electric, magnetic, laser and so on. All of the event data output from these boards are collected by DAQ-Middleware [1], which is the standard DAQ software in J-PARC/MLF. By using this DAQ system, we can analyze all event date with the single clock. And then, we will be able to multi- dimensionally analyze time-transient measurements combined the several conditions of the sample environment or the neutron optics.

In this presentation, we will show the details and applications of our DAQ system.

[1] K. Nakayoshi, Y. Yasu, H. Sendai, E. Inoue, M. Tanaka, S. Sato, S. Muto, J. Suzuki, T. Otomo, T. Nakatani, T. Ito, Y. Inamura, M. Yonemura, T. Hosoya and T. Uchida, Nucl. Instr. and Meth. A623 (2010) 537-539

# Development of New Special Environment Powder Neutron Diffractometer, SPICA

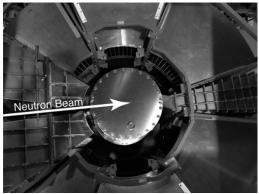
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Batteries are very notable technology in this world. They are used as power storage systems for smart phones, tablet pad, laptop PC, and *etc*. Lifestyle transformations have been provided by appearing new batteries system because these electronic devices are powered by batteries. For next ecological lifestyle, more high-capacity and long-life batteries are required by electric and hybrid vehicles. To support the development of new generation batteries, we decided to install a new dedicated neutron diffractometer for batteries in J-PARC.

SPICA, a new special environment powder neutron diffractometer, is built up at BL09 in MLF/J-PARC. This instrument is optimized for *in situ* measurements of batteries. The SPICA instrument is located 52 m far from the poisoned and decoupled moderator. The maximum diameter of the sample space is 2 m. These unique geometries mean the measurements can be performed in realistic environment with external variables such as temperature, electric field (current density, pulsed current, and *etc.*), high pressure under time-resolved conditions. The over 1600 <sup>3</sup>He gas PSD (Position Sensitive Detector) are arranged on a cylindrical locus from 2 theta = 175 to 10 degrees (See. Fig.1). These detectors have an active length of 0.6 m and are positioned at 2 m from the sample. Neutron guide tubes were selected to have the elliptical arrangements in order to transport neutrons to the sample position and increase the beam intensity without losing the resolutions.

The commissioning of SPICA was carried out in the middle of June 2012 for 2 weeks. The instrumental parameters and several diffraction patterns were collected and verified these are consistent with the instrumental design. The current status of SPICA will be reported.



<u>Figure 1</u>: Detectors layout of the <u>SPICA</u> instrument. Neutron beam is transported from left side. The sample vacuum chamber can be removed.

# Development of New Rietveld Code as Powder Diffraction Analysis Suite, Z-Code

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New Japanese Spallation Neutron Source (JSNS), Materials and Life Science Facility (MLF) in Japan Proton Accelerator Research Complex (J-PARC) has been inaugurated. Six different powder diffractometers (Super High Resolution (S-HRPD), High Throughput (iMATERIA), Engineering (TAKUMI), Total Diffraction (NOVA), Pressure(PLANET) and Special Environment(SPICA)) have already put out the first great data. In this situation, new powerful and useful analysis software for powder diffraction data is desired. Since 2004, the powder diffraction group in J-PARC has started to develop a new powder diffraction analysis suite, Z-Code (code-name for the development). It is the integrated environment for finding out crystal structures using various analysis methods from powder diffraction data. For example, It has the general functions of Indexing, Peak Searching, Structure Matching from a Data Base, and Conventional Rietveld analysis. Z-Code also supports Texture analysis, Profile analysis, Fourier synthesis, and Maximum Entropy Method as the advanced analysis components.

We just released and began to test the new Rietveld analysis software called "Z-Rietveld" with the first users of the powder diffractometers in J-PARC. Z-Rietveld is the one component of Z-Code. It has a Graphical User Interface (GUI) and many powerful features for the refinement of crystal structures. Z-Rietveld has demonstrated nice refinements of a complicated structure models using multiple data sets, such as x-ray and neutron ones. In this presentation, more features and details of Z-Rietveld will be discussed.

## Current Status of Extreme Environment Single Crystal Neutron Diffractometer SENJU at J-PARC

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SENJU is a new single crystal time-of-flight neutron diffractometer installed at MLF of J-PARC. SENJU is designed for precise crystal and magnetic structure analyses under multiple extreme environments such as low-temperature, high-pressure and high-magnetic field. SENJU is also designed for taking diffraction measurements of small single crystals less than 1.0 mm<sup>3</sup> in volume. Construction of SENJU was completed on March 2012 and subsequently, diffraction images of several organic and inorganic crystals such as NaCl, ruby and sucrose were measured at room temperature. In these measurements, Bragg reflections in the high-Q region (d-spacing < 0.5 Å) were successfully observed. On December, diffraction measurement of a laboratory X-ray size single crystal of taurine (\begin{aligned} 0.6 \text{ mm}; 0.1 \text{ mm}^3 \end{aligned}) was carried out (Fig. 1), and the obtained data set were successfully analyzed. Measurement time was 6 days (270kW) and final *R*-factor was 7.16%. Diffraction measurements using a 4K cryostat were also carried out. Diffraction measurements of a TbCoGa5 crystal which shows antiferromagnetic ordering blow 35 K, were carried out at 50 K and 10 K. Magnetic Bragg reflections derived from the ordering were clearly observed at 10 K.



Figure 1 Diffraction image of a 0.1 mm<sup>3</sup> taurine single crystal.

### Development of TOF imaging system with a combination of a neutron image intensifier and a high speed camera

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A high speed imaging device combined with a neutron image intensifier (I.I.) and a high-speed camera is developed for energy resolving neutron transmission measurement with higher spatial resolution and wider vision. The image recording system for time-of-fright (TOF) spectra is adapted to pulsed neutron from an accelerator. The periodic exposure of the camera starts by an electrical pulse which is generated in synchronization with the accelerator, and several tens of TOF images are taken between them. Moreover, we constructed the recording system which can add their TOF images for each time channel automatically to save data-processing capacity of the control PC. As an advantage of this development, long time recording becomes possible.

In our imaging system, transmitted neutron is converted to visible ray by neutron I.I. (Ultimage<sup>TM</sup>nγ-04, Toshiba) at first. Then, it is reflected to optic system contains the camera in the neutron shield by a mirror. The optic system is consist of Fiber Optic Plate (FOP) which can transfer an image without using a lens, the second I.I. for visible light (C9016-02, Hamamatsu) and high-speed CMOS camera (MC1362, Mikrotron) from the upstream. An alignment of these parts allows us to adjust the size transmission

image on the FOP, caught by the camera. The recording system can be selected image size from  $250\times250$ ,  $300\times300$ ,  $500\times500$  and  $1000\times1000$  pixels, however the number of available TOF channels decreases with larger image size. Therefore, we need to choose appropriate condition for the experiment (higher spatial or higher time resolution).

The operational experiment for this imaging system was carried out at the Hokkaido University 45 MeV electron liniac which is equipped the solid methane cold neutron source and it can supply pulsed neutron with 50 Hz. The flight path length from the source to the neutron I.I. was 5.15 m. In this experiment, the exposure time per one TOF channel was decided to 200 µsec and the number of TOF channel was 45. Therefore, a measurable time channel was until 9 msec and it is corresponding to about 6.9 Å in neutron wavelength. The image size was chosen to the smallest 250×250 because of the hardware limit of this device. Metallic plates of Fe, Pb and Cu were used as samples, and their thicknesses were 15, 12 and 8 mm, respectively.

Fig.1 shows the neutron transmission image at 1st TOF channel (left) and 27th (right) on behalf of later channels, which are normalized by the images taken without the metallic plate samples under the same experimental conditions. There is a large difference on Pb area between them. The 1st image was exposed immediately after the electron irradiation to the target by the accelerator, therefore it isn't influenced by only neutron but also prompt  $\gamma$ -ray generated at the target, unlike subsequently taken images. This is coincident with the fact that Pb has lower neutron cross section and enough shielding ability against for  $\gamma$ -ray radiation compared with Cu and Fe.

Fig.2 shows the wavelength dependence of transmitted neutron intensity in the area of Fe, Cu and Pb metallic plates. There is a clear dip at around 4.0 Å in Fe and a small one in Cu. It is conceivable that these dips are originated in the Bragg edge of Fe and Cu, respectively. The Bragg edge of Pb is not appeared in Fig.2 because of its small neutron cross section. Wide TOF images and spectra from which we can discriminate the Bragg edge were obtained by this experiment.

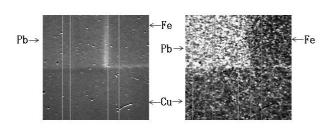


Fig.1 Normalized neutron transmission images at 1st TOF channel (left) and 27th (right).

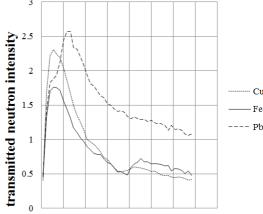


Fig. 2 Wavelength dependence of transmitteed neutron intensity of metalic plates of Fe, Pb and Cu

# Numerical study of MAGIC chopper performance by Monte Carlo simulation

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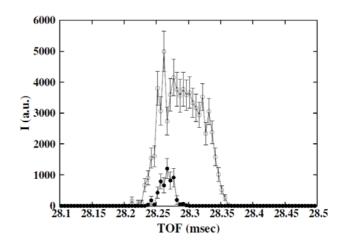
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As an effective device for utilizing multiple incident energies on a chopper spectrometer, a new type Fermi chopper which has neutron supermirrors tucked into its slit package, namely MAGIC chopper, was suggested [1]. In order to design a component of the MAGIC chopper especially for Fermi chopper spectrometer 4SEASONS installed at J- PARC, we demonstrate a numerical simulation of MAGIC chopper performance by Monte Carlo method. Neutron transmittance of a Fermi chopper with and without 3Qc neutron supermirror was calculated. Slit width of 150 mm and length of 17 mm were modeled as a slit package of the Fermi chopper. Rotating frequency was assumed to be 100 Hz. Figure 1 shows the time-of-flight (TOF) spectra of transmitted intensities from rotating slit packages with and without neutron supermirrors. As shown in Figure 1, the intensity gain of MAGIC chopper is found to be significant. It is also demonstrated that the MAGIC chopper can widen the chopper opening time effectively in the longer- TOF region. In this presentation, we will discuss the optimized design for the MAGIC chopper based on the simulation results.

Figure 1. TOF spectra of the MAGIC chopper (open circle) and mirror-less Fermi chopper (solid circle).

[1] M. Nakamura, M. Arai, R. Kajimoto, T. Yokoo, K. Nakajima, and TH. Krist, Journal of Neutron Research, **16** 87-92 (2008).



### A Cold-Neutron Disk Chopper Spectrometer, AMATERAS

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AMATERAS is a cold-neutron disk-chopper-type spectrometer at Materials and Life Science Experimental Facility of J-PARC (Fig.1). By using a series of high-speed disk-choppers and owing to the high peak intensity from a coupled moderator source at MLF, AMATERAS realizes both high-intensity and fine and flexible energy resolution measurements in quasielastic and inelastic neutron scattering experiments from cold to thermal neutron energy region. [1, 2] In our presentation, we will show the over view of AMATERAS including some of examples of recent scientific outputs.

- [1] K. Nakajima et al., J. Neutron Res. 15, 13 (2007).
- [2] K. Nakajima et al., J. Phys. Soc. Jpn. 80 SB028 (2011).



Fig. 1 AMATERAS, a cold-neutron disk chopper spectrometer at MLF, J-PARC.

### Current Status of the Small and Wide Angle Neutron Scattering Instrument (TAIKAN) of J-PARC

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The small and wide angle neutron scattering instrument, TAIKAN, was installed on BL15 in the Materials and Life Science Experimental Facility (MLF) of J-PARC. TAIKAN is designed for efficient measurement in wide-q range of  $0.005 \sim 20$  [Å<sup>-1</sup>]. The 1040 <sup>3</sup>He-PSD tubes with 8 mm in diameter and gas pressure of 6 atm are mounted on four detector banks of small-, middle-, high-, and backward-angle. Fig. 1 shows the photograph of small- and middle-angle detector bank from the front flange of TAIKAN's vacuum chamber. The two detector banks in the chamber are surrounded by the B<sub>4</sub>C shielding boards, in order to avoid the crosstalk between facing detectors and reduce the background.

On-beam commissioning was started in January 2012, and user program has begun since March 2012. We will report on the results of some standard samples, the instrument performance, and the current status of TAIKAN.



Fig.1: Photograph of detector banks (small- and middle-angle) in TAIKAN's vacuum chamber.

# Present Status of a New Pulsed Neutron Imaging Instrument at J-PARC

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We are now constructing a pulsed imaging instrument at beam line 22 in MLF (Materials and Life Science Experimental Facility) of J-PARC (Japan Proton Accelerator Research Complex). This is the world first instrument dedicated to the pulsed neutron imaging, which enable us to make two dimensional image of the crystalline structure and nuclide composition and magnetic fields using the features of the pulsed neutron [1-3]. This instrument also has capability to give the high-resolution images using a higher L/D option compared with other facilities in Japan.

In this presentation, we introduce the current status of the instrument development and the prospective practical researches.

- [1] H. Sato, T. Kamiyama, Y. Kiyanagi, Materials Transactions, Vol.52, pp.1294-1302, (2011)
- [2] T. Kai et.al., Nuclear Instruments and Methods A, 651, 126–130 (2011)
- [3] T. Shinohara et.al., Nuclear Instruments and Methods A, 651, 121-125 (2011)

# Current Status of a newly developed Polarized Neutron Reflectometer (Sharaku) at bemaline BL 17 of J-PARC

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As a nondestructive technique, neutron reflectivity brings significant information on the magnetism at interfaces even in thin films. We constructed a newly developed polarized neutron reflectometer at BL17 SHARAKU installed at MLF, and started the user program in the end of January 2012. The magnet with high field and the spin polarization apparatus are available. We report the current status and future prospects of the beamline in terms of a commissioning and a research.

The collaborators for the construction and the commissioning of BL17 are as follows;

M. Takeda(Leader), D. Yamazaki(sub-Leader), K. Soyama, R. Maruyama, H. Hayashida, M. Kubota, H. Asaoka, T. Yamazaki, K. Aizawa, T. Kamiyama, M. Arai, Y. Inamura, K. Kaneko, T. Nakamura, T. Nakatani, K. Oikawa, K. Sakasai, T. Shinohara, K. Suzuya, I. Tamura, K. Toh, H. Yamagishi, N. Yoshida, Y. Sakaguchi, T. Mizusawa, T. Itoh, T. Ohhara, J. Suzuki, and T. Hirano.

# Quantitative evaluation of nuclide density distribution in a substance using the neutron resonance absorption spectroscopy at J-PARC/MLF/BL10

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The neutron resonance absorption spectroscopy (N-RAS) is the technique of a combination of prompt gamma ray measurement (or neutron transmission measure- ment) and a time-of-flight method. Using the technique we can distinguish nuclides or isotopes and obtain the information of atomic density and dynamics. The observed resonance peak is expressed by convolution of intrinsic resonance and neutron emission time distribution from moderator. To perform quantitative analysis of resonance peak, the emission time distribution must be reproduced at arbitrary neutron energy by synthetic functions. The functions expressing the time distribution (pulse) of J- PARC/MLF/BL10 have not been considered until now. Therefore, we have aimed to make a synthetic pulse function suitable to BL10. As an example, we evaluated atomic number density of Ta foil by N-RAS.

Firstly, we calculated the emission time distributions of epithermal neutron at BL10 by simulation and fitted several kinds of pulse functions to them. We found that the Cole-Windsor function well reproduced the time distribution at arbitrary energy. Next, we implemented the pulse function in resonance shape analysis code "REFIT[1]" to analyze the resonance peaks. As an example, we analyzed the resonance dip in the time-of-flight spectrum due to the resonance of Ta sample with a thickness of 0.01 mm (area density:  $5.48 \times 10^{-5}$  atoms/barn). Fig.1 shows the resonance dip due to 4.28 eV Ta resonance and the result of fitting using REFIT code. By fitting a simulation result to the experimental one using the REFIT code, we obtained a thickness of 0.01 mm ( $5.48 \times 10^{-5}$  atoms/barn) within an error of  $\pm 0.44\%$ . We succeeded to synthesize the pulse function and to evaluate the nuclide density by N-RAS.

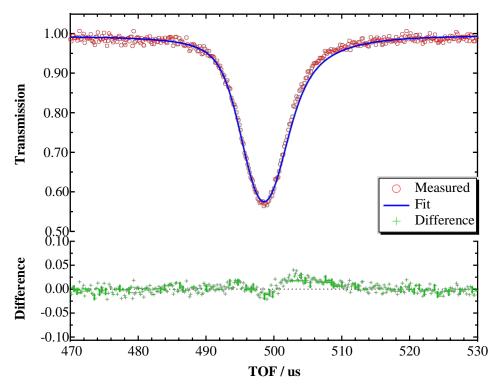


Fig. 1 The resonance dip due to 4.28 eV Ta resonance and the result of fitting using REFIT code.

[1] M.C. Moxon and J.B. Brisland, "GEEL REFIT, A least squares fitting program for resonance analysis of neutron transmission and capture data computer code", AEA-InTec-0630, AEA Technology (1991)

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# NR Studies on the Stimuli-Triggered Changes in Polymer Thin Films with Different MWs

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Stimuli-responsive polymeric thin films based on polyelectrolyte (PE) multilayer thin films and polymer brush platforms with active moieties have received significant attention for many potential applications. In the present study, we prepared multilayer thin films containing a cationic weak PE, linear poly(ethylene imine), and an anionic weak PE, poly(methacrylic acid) with different molecular weights (MWs) in order to investigate the effect of MW on the external pH-triggered release of model multilayer platforms. Well-defined internal structure of the model stimuli-triggered release platforms was obtained by the spin-assisted layer-by-layer (LbL) deposition [1]. Despite the difficulty in detecting the nanometer-scale internal changes of the multilayer films, we have monitored the pH-induced delamination or release of target deuterated PMAA chains with different MWs and corresponding viscoelastic properties of the multilayer films using neutron reflectivity (NR) as well as quartz crystal microbalance with dissipation (QCM-D).

In addition, for further research on NR, structural changes of reactive polymer brush platforms prepared by the surface reversible addition–fragmentation chain transfer (RAFT) polymerization with pentafluorophenyl acrylate monomer [2] are investigated with NR. The reactive ester moieties can be easily modified to impart functions to the polymer brush films by the simple post-polymerization modification with primary amines. We now work on clarifying the reaction mechanism of the RAFT-polymerized brush platforms by monitoring the brush profile along with the concentration gradient of amine-penetration as a function of MW and grafting density of the polymer brushes.

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[2] J. Choi, P. Schattling, F. D. Jochum, J. Pyun, K. Char, and P. Theato, *J. Polym. Sci. Part A: Polym. Chem.*, 50, 4010 (2012)

# SANS Studies on the Effect of Additives on the Morphology of Organic Solar Cells

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Organic photovoltaics (OPVs) have attracted much attention as lightweight, low-cost, and easy to process replacements for inorganic counterparts. Despite recent rapid developments in OPVs, the OPVs still suffer from the low device performance compared with inorganic counterparts due to their short exciton diffusion length as well as low charge mobility. In order to overcome these problems, there have been reports on using self-organized poly[3-hexylthiophene]s (P3HT), called as P3HT nanowires, to create continuous pathways and also to enhance the crystallinity of active layers. However, there is lack of studies on the phase size of phenyl-C61-butyric acid methyl ester (PCBM) surrounding the P3HT nanowires. In the present study, we report the effect of additives on the BHJ morphologies, which could enhance the P3HT crystallinity as well as varying the size of the PCBM phase. We employed a new additive, which has better solubility for PCBM while keeping the solubility for P3HT low in the blend solution. We performed the small angle neutron scattering (SANS), which has the spatial resolution ranging from a few to thousands of nanometers to characterize the nano-morphologies of P3HT:PCBM blends to address the effect of the addition of additives. The SANS results showed that by keeping the P3HT solubility low in the blend solution, higher P3HT crystallinity was achieved. At the same time, the increase in the PCBM solubility led to smaller nanodomains of PCBM agglomerates. Based on the morphological variations by adding additives, P3HT:PCBM BHJ solar cell devices were fabricated and the maximum power conversion efficiency of 3.24% was achieved with the addition of an additive, which is the 43% enhancement when compared with the reference sample without additives.

### Dynamics of PEO Chain in Micro-phase Separated Structure Formed by Liquid-crystal Amphiphilic Di-block Copolymer

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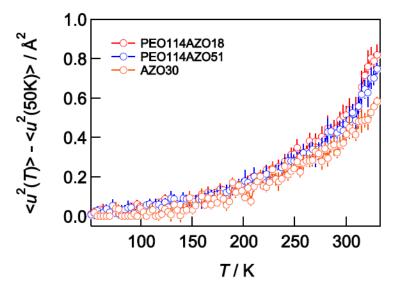
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PEO-AZO amphiphilic di-block copolymer [1] which consists crystalline PEO and side-chain liquid-crystal having azobenzene moieties as a mesogen polymethacrylate derivatives (AZO) forms well ordered hexagonal PEO cylinder structure in wider volume range than that of a linear block copolymer. We clarified that the PEO crystallization and melting temperature is lower than that of bulk PEO chain and that the phase transition temperature of AZO domain is almost the same as that of AZO homo polymer by DSC measurements. This means the dynamics of PEO chain is restricted in the cylinder by size and/or anchor effects. In this study, the dynamics of PEO chain was investigated by quasi-elastic neutron scattering technique. The figure shows mean square displacements (<u²>>) of PEO114AZO18, PEO114AZO51 and AZO30 as a function of temperature. The <u2> of PEO114AZO18 and PEO114AZO51 was jumped around 320 K corresponding to the PEO melting. The comparison with PEO homopolymer will be discussed in the presentation.

[1] S. Asaoka, T. Uekusa, H. Tokimori, M. Komura, T. Iyoda, T. Yamada, and H. Yoshida Macromolecules, 44, 7645 (2011)



# Chain dimension of ring polystyrenes in solutions studied by SANS

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Ring polystyrenes (PSs) were synthesized by anionic polymerization technique and purified with preparative size-exclusion chromatography (SEC). Seven ring PSs with their weight average molecular weight ( $M_W$ ) ranging from 17k to 570k were prepared and they were confirmed to have high purities all over 96% by liquid chromatography at the chromatographic critical condition (LCCC) analyses. Their radii of gyration ( $R_g$ s) were determined in benzene- $d_6$  as a good solvent and in cyclohexane- $d_{12}$  or cyclohexane- $h_{12}$  as theta solvents by small-angle neutron scattering (SANS) or light scattering (LS). It has been found that  $R_g$ s of ring polymers are scaled with  $M_W$  as  $R_g \propto M_W^{0.61}$  in a good solvent (Figure 1a) and as  $R_g \propto M_W^{0.53}$  in theta solvents (Figure 1b). Moreover it was confirmed that g factors,  $R_g^2(\text{Ring})/R_g^2$  (Linear), obtained in theta solvents are meaningfully larger than theoretically predicted values owing to the topological effect stored in ring molecules.[1]

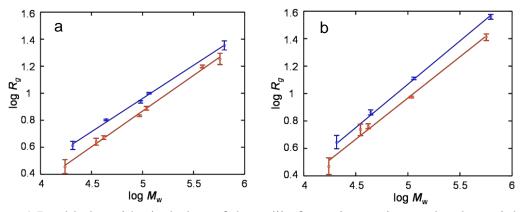


Figure 1 Double logarithmical plots of the radii of gyration against molecular weight for ring (red line) and linear polymers (blue line) (a) in benzene-d<sub>6</sub> and (b) in cyclohexane-d<sub>12</sub>/h<sub>12</sub>.

[1] A.Takano, Y.Ohta, K.Masuoka, K.Matsubara, T.Nakano, A.Hieno, M.Itakura, K.Takahashi, S.Kinugasa, D.Kawaguchi, Y.Takahashi and Y.Matsushita *Macromolecules* **2012**, *45*, 369-373

### Chain dimension of ring polystyrenes in bulk studied by SANS

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A series of ring polystyrenes (PSs) were synthesized by anionic polymerization technique and purified with preparative size-exclusion chromatography (SEC). Four pair of hydrogenous ring PSs (PS-h8s) and also deuterated ones (PS-d8s) with the molecular weight ( $M_W$ ) ranging from 16k to 380k were prepared and they were confirmed to have high purities all over 95% by liquid chromatography at the chromatographic critical condition (LCCC) analyses. Their radii of gyration ( $R_g s$ ) of ring PS mixtures of PS-h8 and PS-d8 with the same  $M_W$  were measured in bulk by small- angle neutron scattering (SANS). It was found that  $R_g$  of ring PSs in bulk is scaled with  $M_W$  as  $R_g \propto M_W^{0.39}$  during the molecular weight range (Figure 1). The result is in good agreement with computer simulations and theoretical predictions.[1]

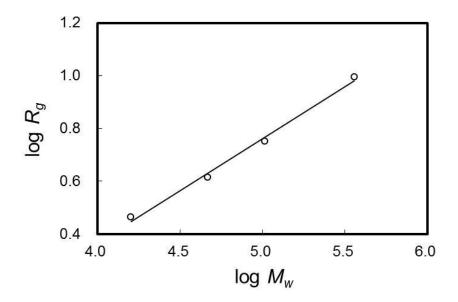


Figure 1 Double logarithmical plots of the radii of gyration against molecular weight for ring polymers in bulk.

#### [1] Takano, et al. Macromolecules to be submitted

### Calculation of Space-time Correlation Function on Liquid Benzene by using MEM

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Dynamic structure factor,  $S(Q,\omega)$ , which can be obtained by neutron scatterings is defined as a Fourier-transformed function from van Hove's space-time correlation function, G(r,t), which is a function in real space and time. G(r,t) is important for elucidation of relaxation phenomena to express the motion of atoms and molecules directly. However, the calculation of G(r,t) has been hardly performed even though it is so easy mathematically, because it was difficult to measure both in high resolution and wide Q-E range. By the progress of the recent neutron sources and spectrometers, the measurements with wide range and high resolution in Q-E space are becoming easy. We measured high-resolution  $S(Q,\omega)$ 's using AMATERAS spectrometer installed at J-PARC and calculated G(r,t)'s. We chose benzene and benzene-d6 as the samples, which were simple molecular liquids. We used the maximum entropy method (MEM) to lower the bias of truncation errors for the calculation of G(r,t). Figure shows the calculated G(r,t) of benzene at 279K. Because G(r,t) includes the self-correlation term, the intensity of G(r,t) is represented as  $I(r,t) 4r^2G(r,t) \square \square$ .

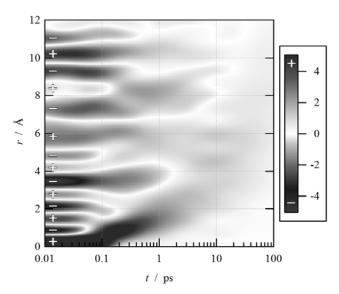


Fig. Space-time correlation function of liquid benzene at 279 K.

# Moisture effect on Double network polymers using J-PARC/TAIKAN(BL15)

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Moisture effect of mechanical properties against dried aqueous polymer network was experimentally discussed. A freeze-dried Double network hydrogel (DN-gels<sup>1</sup>) increases Young's modulus and fracture stress in range of relative humidity (RH) from 0 to 30%. When RH exceeds 30%, with increasing RH, elongation of the samples could be observed. Under the RH between 0 to 80%, the humidity reversibility can be observed. When RH exceeds 80% (water content is about 17wt %), the water content in the network abruptly increased and the Young's modulus abruptly decreased. Focusing on the behavior of water located onto the polymer chains, we approached thermodynamic approach (differential scanning calorimeter), spectroscopic approach (Infrared, nuclear magnetic resonance), and structural approach (wide angles X-ray scattering, and small angle neutron scattering).

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# Study of direct relations between the spiral spin ordering and electric polarization in Mn<sub>1-x</sub>Co<sub>x</sub>WO<sub>4</sub>

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Magnetoelectric multiferroics refer to materials that ferroelectricity (ferro)magnetic spin orders are simultaneously observed, and often exhibit strong coupling. Such coupling between (ferro)magnetic and ferroelectric order is known as magnetoelectric effect. MnWO<sub>4</sub> is one of the best studied magnetoelectric multiferroics. In this material, ferroelectric polarization (P) is observed only in the elliptical spiral incommensurate antiferromagnetic spin order (AF2 phase,  $T = 7.6 \sim 12.7$  K, the **P** is parallel to the b axis), but not in the collinear commensurate (AF1 phase, T < 7.6 K) or the collinear incommensurate (AF3 phase,  $T = 12.7 \sim 13.5$  K). The major direction of the ferroelectric polarization on the AF2 phase can be explained based on the spin current model, i.e.  $\mathbf{P} = A\mathbf{e}_{ii} \times (\mathbf{S}_i \times \mathbf{S}_i)$ .

We investigated the Co doping effect on magnetic spin structures of multiferroic  $Mn_{1-x}Co_xWO_4$  using neutron diffraction experiments. The main results are that the noncollinear spiral AF2 is stabilized down to the base temperature in replacement of the AF1 when the Co substitution increases up to  $x \sim 0.05$ , and the spiral planes of the AF2 becomes perpendicular to the  $\boldsymbol{b}$  axis when  $x = 0.10 \sim 0.15$ . This spin-flop transition is accompanied by the flop of the ferroelectric polarization. For  $x = 0.10 \sim 0.15$ , it is confirmed that the primary orientation of  $\boldsymbol{P}$  is along the  $\boldsymbol{a}$  axis, not the  $\boldsymbol{b}$  axis. For x = 0.20, however, the spiral planes and the main  $\boldsymbol{P}$  direction reverts back to the  $\boldsymbol{b}$  axis. All these results indicate that the magnetoelectricity of  $Mn_{1-x}Co_xWO_4$  can be explained by the spin current model, and it can be controlled via Co doping.

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# Heliconical magnetic ordering and field-induced electric polarization in $Zn_2Y$ and $Co_2Y$ hexaferrites

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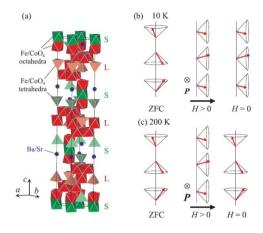
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Hexagonal ferrites containing  $Fe^{3+}$  (S = 5/2) ions exhibit robust magnetoelectric coupling stable near or above room temperature. Hopes are high for device applications exploiting this novel phenomenon, because their magnetoelectric polarization can be controlled at relatively small magnetic fields.

In this work, we investigate the magnetic ordering of two related Y-type hexaferrites, namely Al-doped  $Zn_2Y$  and  $Co_2Y$ , that exhibited field-induced magnetoelectric polarization. Following zero field cooling, we observed incommensurate heliconical magnetic ordering commonly in the two hexaferrites. Upon application of external field perpendicular to the hexagonal c axis, however, commensurate transverse ordering was stabilized in the field range that exhibit magnetoelectric polarization. We argue that the consistent behaviors of the two compounds can be understood based on two coexisting and competing anisotropy fields. [1].



[1] Hak Bong Lee et. al, PRB 86 094435 (2012)

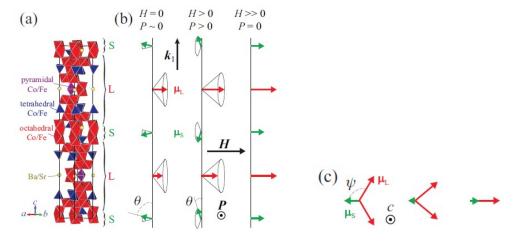
### Single crystal neutron diffraction of magnetoelectric Co<sub>2</sub>Z hexaferrite

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Over the past decade, several types of hexaferrites have been studied with the prospect of achieving high-temperature magentoelectric effect. Such effect at room temperature was finally realized in polycrystalline and single crystalline samples of Co<sub>2</sub>Z-type hexaferrites [1,2].

In this work, we investigated the correspondence between the spin ordering and the electric polarization in the single crystal Ba0.52Sr2.48Co2Fe24O41 under external field. Neutron diffraction data showed that the spin ordering remained to be commensurate to the lattice through the field cycling up to 3 T. The overall field dependence of the magnetic ordering indicated that the transverse conical ordering is directly related to the electric polarization, which is consistent with other types of magnetoelectric hexaferrites. Our work demonstrates that the magnetoelectricity of different hexaferrites can be understood based on the common picture, which involves competing exchange interactions and coexisting two different anisotropies[3].



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- [2] S. H. Chun et al., Phys. Rev Lett. 108, 177201 (2012)
- [3] H. Chang et al., Phys. Rev B. 85, 064402 (2012)

### Neutron scattering studies in non-centrosymmetric superconductors CeTSi<sub>3</sub> (T = Rh, Ir)

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Discoveries of non-centrosymmetric (NCS) heavy-fermion (HF) superconductors CePt<sub>3</sub>Si[1], UIr[2], CeRhSi<sub>3</sub> [3] and CeIrSi<sub>3</sub> [4] draw strong attention as one of the most important topics in the strongly correlated electron physics. The crystal structure of CeTSi<sub>3</sub> (T = Rh, Ir) is the BaNiSn<sub>3</sub>-type belonging to the space group *I4mm* (No. 107) without an inversion center. While both compounds exhibit the antiferromagnetic (AFM) ordering below  $T_N = 5.0$  K and 1.6 K at ambient pressure,  $T_N$  decreases and the superconductivity (SC) appears in a wide pressure range by increasing the pressure. We have been studying CeTSi<sub>3</sub> (T = Rh, Ir) mainly by neutron scattering, to elucidate the correlation between AFM and superconductivity.

- (1) To determine the magnetic structure of both compounds, we performed neutron diffraction experi- ments using the triple-axis spectrometers GPTAS at JRR-3 and HB-1 at ORNL, we observed incommen- surate Bragg reflections below  $T_N$  for both compounds at the propagation vectors of k = (0.215, 0, 0.5) and (0.265, 0, 0.43) for CeRhSi3 [5] and CeIrSi3[6], respectively. From the representation analyses, we found that both compounds exhibit the longitudinal spin-density-wave state (LSDW) with the magnetic moment polarized to a-axis.
- (2) To investigate the nature of the AFM and the SC in these materials, we performed an inelastic neutron scattering experiment on CeRhSi3 using the triple-axis spectrometer IN14 (with the FlatCone multianal- yser) at ILL and observed magnetic fluctuations at low temperatures for the first time. They are broad with the correlation length of  $\xi$ //a-axis ~ 15 Å but  $c^*$ -independent behavior, indicating the magnetic fluctuation in CeRhSi3 is the 2-dimentional character confined in the a-b plane, which is quite contrast to the recent NMR result under SC optimal pressure of 2.7 GPa in CeIrSi3 being the 3-dimensional character.[7] In the meeting, we will discuss the details of the above results.

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## Structure of SiO2-GeO2 glasses by J-PARC NOVA

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